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February 10, 2004

Members of the NSRC Operations Budget Review Committee,

Enclosed are the materials required for review of the FY2006-8 operations budgets for ORNL's ***Center for Nanophase Materials Sciences***, including the detailed staffing plan, the detailed budget, advisory committee memberships and meeting dates, our user policy, and a brief proposal for how 10% additional budget could be spent with great scientific impact and benefit to the national nanoscience user community.

Also contained in this document is supporting material that briefly summarizes scientific challenges and technological opportunities that will be addressed by CNMS, and their relation to its scientific and administrative organization. With strong support from our *Scientific Advisory Committee* (SAC), special attention has been given in the CNMS to the reliable delivery to the user community of a set of unique research instruments and experimental and computational capabilities, as well as opportunities for leadership in nanoscale science using these.

The current scientific and administrative structure of CNMS is the result of a series of interactions that included BESAC (November 14-15, 2001); two well-attended CNMS Planning Workshops with the national scientific community (October 24-26, 2001 and June 23-25, 2002); several small workshops on specific scientific topics; continuing close interaction with the SAC; and several DOE design reviews leading to authorization to proceed with construction and acquisition of technical equipment, which is currently underway. The CNMS building, located on ORNL's new *Spallation Neutron Source* (SNS) campus, is scheduled for completion at the beginning of April 2005, slightly more than one year from now.

We look forward to meeting with you in Rockville for the CNMS Operations Budget Review on the morning of February 19.

With all best regards,

Doug Lowndes, CNMS Director

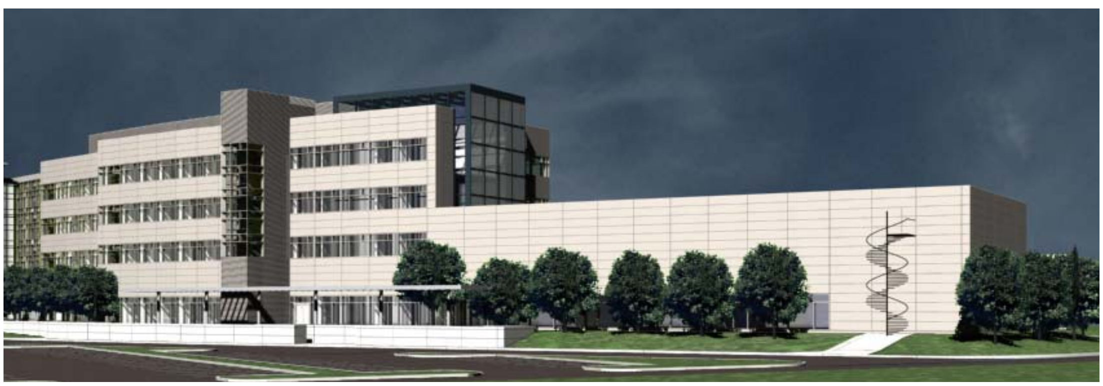
Linda Horton, CNMS Project Manager and Deputy Director

DOE Review of the Operating Budgets of the NSRCs

REQUIRED AND SUPPORTING REVIEW MATERIALS

CENTER FOR NANOPHASE MATERIALS SCIENCES
Oak Ridge National Laboratory

Doug Lowndes, Director
Linda Horton, Deputy Director



Rockville, MD
February 19, 2004

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I. Introduction: The CENTER FOR NANOPHASE MATERIALS SCIENCES

I.1 CNMS Mission and National Needs

Oak Ridge National Laboratory is developing, in partnership with the national scientific community, a highly collaborative and multidisciplinary ***Center for Nanophase Materials Sciences*** (CNMS). The CNMS will be located together with the ***Spallation Neutron Source*** (SNS) and the ***Joint Institute for Neutron Sciences*** (JINS) on ORNL's SNS "new campus." This location supports the recognition, by the Interagency Working Group on Nanoscale Science, Engineering, and Technology (IWGN), of the importance of co-locating new DOE Nanoscale Science Research Centers (NSRCs) with major national facilities for neutron and x-ray scattering. The SNS is expected to become the world's leading neutron scattering facility for studying the structure and dynamics of materials. The CNMS will provide urgently needed capabilities for the synthesis and characterization of nanoscale systems; for nanofabrication; for theory, modeling, and simulation; and, through these, for nanomaterials design. It will bring together and create synergies among these areas in which the United States has clear national needs, and will utilize the unique neutron scattering capabilities at SNS, as well as extraordinary computational resources being developed through ORNL's *Center for Computational Sciences* (CCS), to understand nanoscale materials and phenomena.

The scientific vision for CNMS is to create a user research environment that will accelerate the pace of scientific discovery and drive technological advances. We will accomplish this by assembling the best ideas and the best instruments and by capitalizing on ORNL's unique strengths, in a way that will meet the Challenge issued by BES for the new NSRCs: to "maximize resources and promote multidisciplinary interactions, in order to enable research of a scope and depth beyond current national capabilities."

The scientific organization of the CNMS has evolved over the past two years in a way that directly supports the mission of the Office of Science, "To advance basic research *and the instruments of science* that are the foundation's for DOE's applied missions, a base for U.S. technology innovation, and a source of remarkable insights into our physical and biological world and the nature of matter and energy." With the strong support of its Scientific Advisory Committee (SAC), the CNMS will make *reliably* accessible to the national user community a number of *unique* new nanoscience research instruments, especially emerging neutron scattering and computational nanoscience capabilities. We note that the very definition of nanoscience as "discovering the rules *and developing the tools* needed to fully exploit the benefits of nanotechnology" requires this emphasis, and also maps directly onto the Office of Science Mission.

I.2 Building and Initial Technical Equipment

As of February 1, 2004 construction of the new CNMS building was 14.8% complete, within budget, and on schedule for completion and beneficial occupancy in April 2005 (CD-4a). The overall project completion and full operation date is September 2006 (CD-4b, including installation and operation of the initial technical equipment set).

For the convenience and orientation of the Review Committee, Appendix A provides a simplified summary of the layout of associated groups of laboratories over the four-level office and laboratory building and the connected single-level *Nanofabrication Research Laboratory* and clean room. Appendix B lists the initial technical equipment set that is part of the CNMS Project.

I.3 **Advisory Groups**

The CNMS utilizes four different advisory groups in its governance: a Scientific Advisory Committee (SAC); a Proposal Review Committee (PRC); a Users Executive Committee (UEC); and, an ORNL Management Integration Team (MIT). Relationships among the first three external groups and the upper part of the CNMS' management structure are shown in the CNMS organization chart in Fig. 1. Planning for the CNMS within ORNL has been coordinated and carried out since the pre-proposal stage with guidance from a CNMS Scientific Leadership Team whose activities are described in section I.5 of this document, which describes the CNMS Management Plan.

Scientific Advisory Committee

Invitations to serve on the CNMS' first SAC were issued in the spring of 2003. The initial SAC consists of six external members and three interim ORNL members, as follows:

Jerzy Bernholc (North Carolina State University)
Jack Crow, Chair (National High Magnetic Field Laboratory and Florida State University)
Mostafa El-Sayed (Georgia Institute of Technology)
Dan Morse (University of California, Santa Barbara)
Rick Smalley (Rice University)
Julia Weertman (Northwestern University)
Linda Horton (CNMS Project Director, ORNL)
Thom Mason (SNS Director, ORNL)
Malcolm Stocks (ORNL)

The three ORNL members of the SAC are appointed to serve during the CNMS construction period. They provide the external members with the most recent information—including planning information—on construction and development of the SNS and on the evolution of the computational facilities for ORNL's *Center for Computational Sciences* (CCS), both of which will be particularly important to CNMS users. The three interim ORNL members will leave the SAC before operations begin at CNMS in FY2006.

At least five new members, all external to ORNL, will be added to the SAC during the coming year in order to provide additional guidance in particular areas. The additional members will include experts in nanofabrication; in "unique instruments" development and operation (a SAC recommendation); a theorist; and at least one member from another NSRC. In addition, the Chair of the User's Executive Committee will join the SAC as an ex officio member as soon as the UEC is functioning.

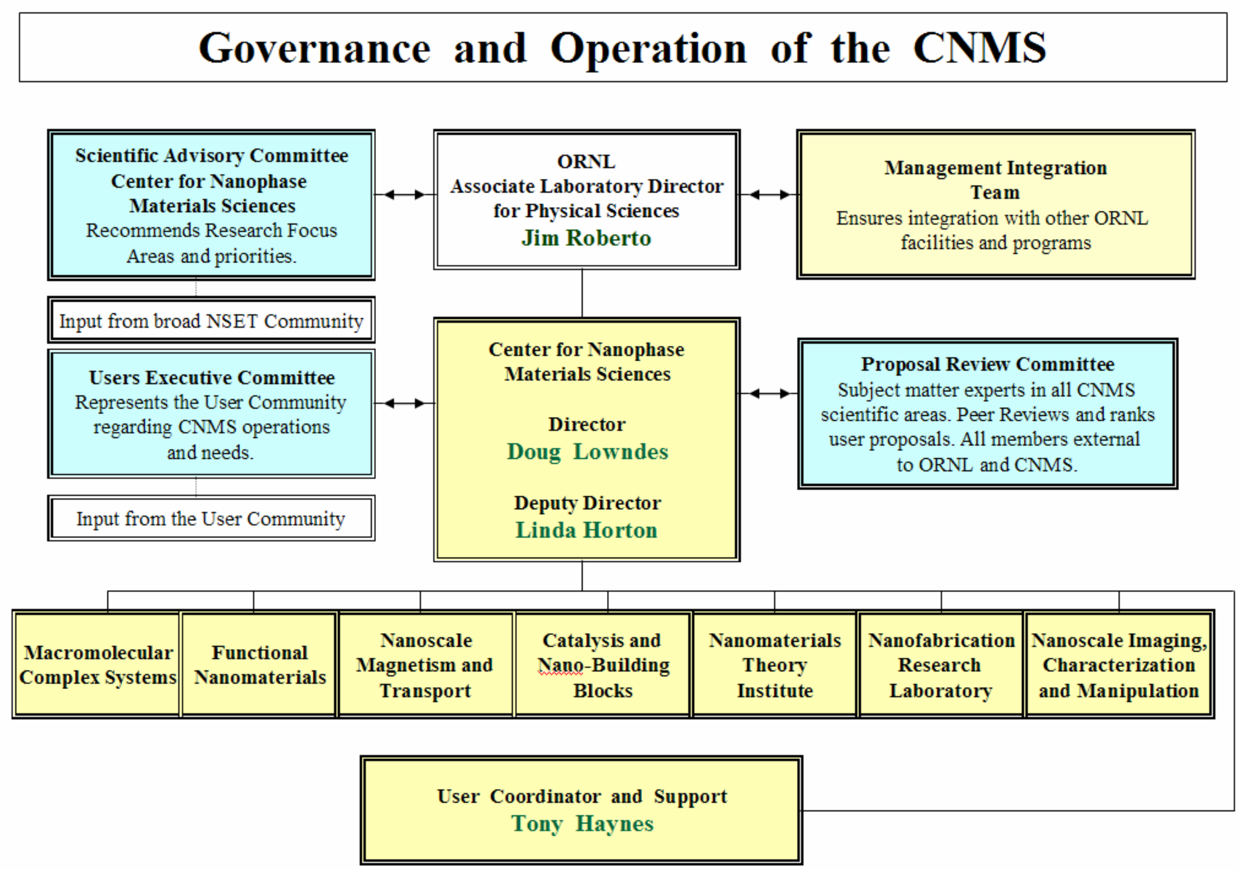

Figure 1. CNMS organization chart.

<u>First SAC Meeting</u>. The first SAC meeting was held June 19–20, 2003 in Oak Ridge. The CNMS' scientific organization and plans for its development were described in presentations by Doug Lowndes, Michelle Buchanan, Peter Cummings, Mike Simpson, and Ward Plummer. The CNMS' construction project and technical equipment set were reviewed by Linda Horton, while the user program and "jump start" Call for Proposals were described by CNMS User Coordinator Tony Haynes. The SAC issued a Report including recommendations (see discussion in Section I.4 of this document, Scientific and Operational Organization of the CNMS).

<u>Second SAC Meeting</u>. In late January–early February of 2004, the SAC again was convened in order to review preparations for this Operations Budget Review. Draft documents were sent to SAC members by express delivery and e-mail attachment, and a 2-hour telephone conference call meeting was held on Feb. 4. In preparing for this meeting, the SAC members were asked particularly to focus on four questions:

(1) Are the numbers and types of positions and facilities adequate to reliably and safely address user research needs in a world-class nanoscience user research center?

(2) Are there appropriate concentrations of unique facilities and expertise to produce major advances in nanoscale scientific understanding (and ultimately nanotechnology)?

(3) Are we investing enough to continuously refresh a state-of-the-art Nanoscale Science Research Center?

(4) Are there other emerging scientific opportunities in which CNMS should play a role because of the available synergies and capabilities?

SAC Recommendations regarding these four issues are presented and discussed in section IV of this document (Scientific Impact of 10% Additional Budget…); in section I.4 (Scientific and Operational Organization); and in Section II, Guiding Principles for CNMS Staffing and Budget.

Proposal Review Committee

CNMS currently has a 14-member PRC that was selected just prior to the July–August, 2003 Call for Proposals to the CNMS jump start user-initiated nanoscience research program. The PRC members are:

Mary E. Galvin (Materials Science and Engineering, U. of Delaware)
Sharon Glotzer (Chemical Engineering, Materials Science and Engineering, and Macromolecular Science and Engineering, U. of Michigan)
Todd D. Giorgio (Biomedical Engineering and Chemical Engineering, Vanderbilt U.)
Steve Granick (Chemical and Biomolecular Engineering, U. of Illinois, Urbana-Champaign)
Robert Hull (School of Engineering and Applied Science, U. of Virginia)
Timothy E. Long (Chemistry, Virginia Polytechnic Institute and State U.)
Marco Buongiorno-Nardelli (Physics, North Carolina State U.)
Phillip E. Russell (Director, Analytical Instrument Facility, Materials Science and Engineering, North Carolina State U.)
Rainer Schad (Physics and Astronomy, U. of Alabama)
Mark A. Shannon (Mechanical and Industrial Engineering, U. of Illinois, Urbana-Champaign)
Susan Sinnott (Materials Science and Engineering, U. of Florida)
Ya-Ping Sun (Chemistry, Clemson U.)
Zhong L. Wang (Director, Center for Nanoscience and Nanotechnology, School of Materials Science and Engineering, Georgia Institute of Technology)
Otto Zhou (Physics and Astronomy, U. of North Carolina, Chapel Hill)

The initial PRC members were selected for their expertise in polymers and bio-inspired materials, carbon nanotubes and related structures, nanoscale imaging, nanofabrication, computational nanoscience, and nanoscale magnetism, all of which are areas in which user proposals were solicited and accepted in the jump start nanoscience user program. Additional members with appropriate expertise will be added to the PRC as the user nanoscience program is broadened, and in order to balance the reviewing load in especially popular research areas.

Users Executive Committee

It is currently expected that a UEC will be formed during FY2005, after the first year of operation of the jump start user program, i.e. as soon as there is a reasonably large user corps, and prior to the beginning of operations in the CNMS building in FY2006.

Management Integration Team

In anticipation of future operations, the CNMS recently formed the Management Integration Team to assist in coordination across ORNL facilities and to ensure equity in the cost-sharing of research staff members. The guiding principle is that cost-sharing must be *entirely appropriate from the perspectives of both the CNMS and other Laboratory units or programs*. This group consists of the leadership of all of the affected Laboratory divisions and DOE programs, as shown in Table 1. Please see the more detailed discussion of research staff cost-sharing in section II.6.

Table 1. Members of the CNMS Management Integration Team (including organizational and programmatic affiliations)

Michelle Buchanan, CSD Director (BES Chemical Sciences)
John Cooke, CMSD Director (BES Condensed Matter Physics and Materials Chemistry)
Linda Horton, BES Materials and Engineering Physics Program Director
Doug Lowndes, CNMS Director
Jeff Nichols, CSMD Director (Office of Advanced Scientific Computing Research)
Jim Roberto, Associate Laboratory Director for Physical Sciences
Thom Mason, Associate Laboratory Director for the SNS
Thomas Zacharia, Associate Laboratory Director for Computational Sciences

(*italics* = members currently also serving on the CNMS SAC)
CSD: Chemical Sciences Division; CMSD: Condensed Matter Sciences Division; CSMD: Computer Science and Mathematics Division.

I.4 <u>**Scientific and Operational Organization of the CNMS**</u>

The CNMS will support a focused research agenda that has been developed together with the national nanoscience research community through two successive CNMS Planning Workshops, one held in late October of 2001, the second in late June of 2002. These workshops received a tremendous response from the national community, e.g., more than 300 participants representing more than 85 institutions took part in the Second CNMS Planning Workshop. The principal work of the workshops took place in a series of Breakout Sessions, in which the participants were asked to define candidate Research Focus Areas for CNMS, together with their equipment needs, while focusing on the greatest challenges to scientific understanding and the greatest opportunities for new technology. Fourteen Research Focus Areas—spanning soft and hard materials, nanofabrication, theory and modeling, and nanomaterials design—were defined, together with a cross-cutting topic on quantum transport in nanostructured materials. Nine of these now are present in the CNMS staffing and budget plan. In addition to the input from the scientific community obtained from the workshops, the CNMS SAC provided guidance and direction. This input is summarized below.

<u>Recommendations from the First *Scientific Advisory Committee* Meeting</u>: In June, 2003 the scientific leadership of CNMS met with its newly appointed SAC for discussion of the scientific program and to obtain recommendations for its development. Two important recommendations of the SAC resulted:

First, that CNMS should begin immediately to *highlight and develop new capabilities that will be world-class*, since these are expected to be the most significant "draw" for new users, and will help stimulate new research opportunities.

Second, that every effort should be made to *engage the scientific community in the development of new capabilities*, since the community has been a significant force driving the development of new capabilities at other national user facilities.

The judicious use of shared postdoc positions and of merit-based graduate student fellowships to support collaborative development of CNMS capabilities also was considered effective.

The SAC's recommendations underline the widespread recognition that there is a growing need for a new generation of experimental instruments and computational tools that both *integrate* and *improve* upon previously separated capabilities. On the experimental side, there is clear need for instrumentation that *combines* nanoscale imaging with new *in situ* properties measurement and sample manipulation capabilities (e.g., contacting, force-application, deposition, cutting), as well as special environments to enable using neutron scattering to understand nanoscale phenomena. On the theory/modeling side, there is a pressing need for computational tools able to address challenges such as multi-scale modeling and, ultimately, the design of functional nanomaterials and systems.

<u>CNMS Organization:</u> The CNMS has been designed to address these instrumentation and computational challenges through two aspects of its organization: First, by supporting user nanoscience research in a set of seven key Scientific Theme areas that resulted from the planning workshop process. These themes are shown in Table 2 and described below. Second, by supporting the development of new instruments and computational methods that *define the state-of-the-art* and—once these are developed—by providing technician and staff support to make these *reliably* available to users. The second objective will be pursued through the CNMS' *Nanomaterials Theory Institute* and under its *Nanoscale Imaging, Characterization, and Manipulation* Scientific Theme. The development of new scanning probe- and electron microscopy-based instruments can be accomplished (1) if there is at least partial support from the CNMS capital equipment budget, (2) by providing support for workshops and/or symposia that result in the formation of teams for development of specific instrumentation, and (3) by utilizing CNMS as a base for national and international collaborations with leading scientists and groups. It should be noted that the research under the *Nanoscale Imaging, Characterization, and Manipulation* Theme is not pursued independently, but in fact addresses the science-driven research needs of users of the other Scientific Themes.

An important result of having the CNMS SAC review the initial draft of this document was to identify where additional budget support could be applied with *disproportionate* scientific impact on nanoscience user research. One of the areas for enhancement is the development of special environments for neutron scattering, in order to utilize the unique capabilities of the SNS. A second suggestion is to provide additional staff for computational nanoscience research, to make the unmatched capabilities at the CCS readily accessible to the national and international nanoscience user community. A final suggestion is to ensure sustainability of the CNMS at the cutting edge by supporting the ongoing development of unique instruments for nanoscience research. The interaction with the SAC and its Recommendations are summarized in section IV of this document.

In the text that follows, CNMS' Scientific Themes are described, followed by an outline of plans for the CNMS suite of unique and state-of-the art nanoscience instruments, computational nanoscience modeling and simulation tools, and nanocharacterization tools.

Table 2. CNMS **Scientific Themes** and staff member(s) expected to have primary **operational** responsibility in the CNMS building (**boldface type**). *Research Focus Areas* (*italics*) and their scientific leadership also are shown. (See Table 3 for Affiliated research areas not located in the CNMS building.)

Macromolecular Complex Systems (Britt)
Synthetic and Bio-Inspired Macromolecular Materials (Britt, Mays)
Nanophase Biomaterials Systems (Simpson, Doktycz)

Functional Nanomaterials (Geohegan, Christen**)**
Nanotubes, Nanowires, Quantum Dots, and Related Nanostructures (Geohegan, Lowndes)
Artificial Oxide Film Structures (Christen, Rouleau)

Nanoscale Magnetism and Transport (Plummer**, Baddorf)**
Magnetism in Nanostructured Materials (Shen, Baddorf)
Quantum Transport in Nanostructured Materials (Baddorf, Kalinin, Pantelides)

Catalysis and Nano-Building Blocks (Overbury, Schwartz**)**
Nanostructured Materials for Highly Selective Catalysis (Dist. Sci. TBD, Overbury, Schwartz)

Nanomaterials Theory Institute (NTI): Theory, Modeling and Simulation (Cummings, Schulthess, Stocks**)**
Virtual Synthesis and Nanomaterials Design (Cummings, Glotzer)
Electronic Structure, Correlations and Transport in Nanostructured Materials (Schulthess, Stocks)

Nanofabrication (Nanofabrication Research Laboratory, NRL) (Simpson / TBD**, Kasica)**
Controlled synthesis and directed assembly to support all CNMS Scientific Themes (Kasica)
Nanophase Biomaterials Systems (Simpson, Doktycz)

Nanoscale Imaging, Characterization, and Manipulation (NICM)
Includes soft and hard materials and new soft-materials techniques
Neutron and X-ray Scattering **(Egami,** Simonson/Myles; (A) Larson/Ice**)**
Special scattering environments and techniques for nanoscience
UHV Scanning Probes **(**Plummer**, Wendelken)**
Nanoscale magnetic and transport properties; in situ monitoring of growth; quantum transport in nanostructured materials (Weitering, Pantelides)
Electron Microscopy and Spectroscopy **(Joy,** Anderson**)**
Electron imaging combined with other characterization and manipulation methods; use of special environments; ambient scanning probes

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I.4.a **Scientific Themes at the CNMS**

The nanoscience research program to be housed in the new CNMS building is outlined in Table 2. As discussed above, the research is organized under 7 Scientific Themes (shown in boldface type). Each Scientific Theme supports two or more of the Research Focus Areas (shown in italics) that were identified through the planning workshop process. Shown in boldface type are the names of the scientists who are expected to have overall operational responsibility for the conduct of research.

Each Research Focus Area (italic type) is led or co-led by one or more internationally known scientists who have responsibility for scientific guidance and development of the area. A number of these internationally known leaders (e.g., ORNL-UT Distinguished Scientists, ORNL Corporate Fellows, and some ORNL Distinguished Members of Research Staff) are *budgeted at only 10%* of their salary support (see Table 5, section III.1, CNMS Staffing). However, these leaders will play a key role in developing the user community and research collaborations on the national level for CNMS, organizing conferences and workshops, and mentoring students and postdocs. In fact—as pointed out by SAC members—for this modest investment in salary support, CNMS is likely to actually obtain much more than 10% of their time.

Beyond the scientific and operational leaders, each scientific area is staffed by research staff members, postdocs, and technicians who will provide research support and collaboration to CNMS users.

In addition to the capabilities located at CNMS, users will have access to affiliated research capabilities located in the SNS Central Lab and Office (CLO) building, the main ORNL campus, or an ORNL beam line at the Advanced Photon Source (Argonne National Laboratory), as summarized in Table 3. These capabilities are not budgetarily part of the CNMS but their existence will be made known to the user community in order to provide limited support for user proposals that are accepted through the peer review process, on an “as available” and “as needed” basis. Finally, CNMS users also will be able to use for nanoscience research other major ORNL User Facilities for which Memoranda of Agreement (MOAs) with CNMS either are in place or being prepared. These User Facilities also are listed in Table 3.

Table 3. Affiliated ORNL research areas and user facilities not located in the CNMS building. (Acronyms: CSD: Chemical Sciences Division; M&C: Metals and Ceramics Division; CMSD: Condensed Matter Sciences Division; LSD: Life Sciences Division; APS: Advanced Photon Source.

Associated Research Focus Areas and locations:
Fluids in Confined Geometries (Cole, CSD, 4500S)
Nanofunctional Bulk Materials: Collective and Interfacial Behavior (Egami, M&C, 4500S, and Becher, M&C, 4550)
Oxide-Semiconductor Nanosystems (McKee, M&C, 4500S)
Synthesis of Functional Nano-Building Blocks (Mandrus, CMSD, 3150)
Synthesis of Functional Nano-Building Blocks (Beach, 4500S, CSD)
Nanoscale and Molecular Mechanics (Thundat, 4500S, LSD)

Support laboratories not duplicated in the CNMS:
Crystal Growth (Mandrus, CMSD, 3150)
Catalysis Laboratories (CSD, 4500S)
Deuteration Facilities (CSD, 4500S; also SNS CLO)
Synchrotron XRD Facilities (Larson/Ice at APS, Argonne)
Advanced Materials Characterization Laboratory (M&C and CMSD; houses aberration corrected electron microscopes)

Other ORNL User Facilities with which CNMS has/will have MOAs:
Center for Computational Sciences (CCS)
Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR)
High Temperature Materials Laboratory (HTML)
Shared Research Equipment Program (SHaRE)

It should be noted that the first six affiliated ORNL research areas in Table 3 correspond to five (of 15 original) candidate research areas from the CNMS Second Planning Workshop. Thus, approximately 1/3 of the candidate research areas have been eliminated because they cannot be supported budgetarily and are perceived to involve smaller numbers of potential users, based on the Second Planning Workshop response. However, in the Feb. 4 discussion of our operating budget, the SAC *strongly cautioned against any further reduction of the CNMS' scientific scope*, pointing out that "the real opportunity to optimize the investment of resources will only come after some years of operating experience, and as the field of nanoscience itself becomes better defined"; that "we can hope to see clearly in five years but to try to guess now may be foolish"; and that scientific breadth is needed initially because "the greatest scientific impact will come from combining your known strengths with the still unknown strengths of the users."

The CNMS' planning workshop process was critically important because it not only enlisted the national community to identify nanoscience research areas in which there are great scientific challenges and technological opportunities, but also those for which there is *a demonstrated high level of demand* for user-initiated research. The Research Focus Areas listed under the first six Scientific Themes provide synthesis, characterization, theory/modeling/simulation, and nanomaterials design support for a significant range of soft, hybrid, and complex hard materials research, as we now outline.

Macromolecular Complex Systems addresses the grand challenge of designing and controlling the nanoscale organization of macromolecular materials. Research will focus on both synthetic and naturally occurring macromolecules, as well as hybrid structures. Directed self-assembly strategies will be used to create hierarchical structures with targeted material properties and/or biological function. This area has strong need for a parallel theory and modeling effort focused on the design of new materials, providing insights into principles governing and relating structure, properties and function, and leading ultimately to theoretical understanding with predictive capabilities. A likely outcome of user-initiated research will be the development of synthetic techniques for the controlled synthesis of macromolecules by living anionic, cationic, and free radical techniques. For neutron scattering studies—a key tool in the characterization of these systems—isotopic labeling techniques will be needed to facilitate custom synthesis of deuterium-labeled polymers. Techniques and expertise will be developed to assist users in the characterization of novel macromolecular architectures in solution, on surfaces, and in the bulk by a variety of methods that include light scattering, small angle X-ray and neutron scattering, NMR, spectroscopic methods, electron microscopy (SEM and TEM), and AFM. There is strong coupling of this area with Functional Nanomaterials, where part of the scientific focus is on synthesis and properties measurements for carbon and other nanotubes, nanorods and related structures, including multifunctional composites.

Functional Nanomaterials addresses several challenges: the controlled synthesis of high quality nanorods, nanowires, and quantum dots of a wide range of materials, and measurements to understand nanoscale effects of size and dimensionality on their properties; the need to develop methods for using these nanomaterials in composites, accompanied by fundamental understanding of nanoscale mechanics and interface science; and the opportunity to collaborate with users in applying new ORNL capabilities for the efficient discovery and synthesis of artificially layered oxide film structures whose magnetic and electric properties can be systematically explored and tuned. Unique capabilities for time-resolved, in situ diagnostics of the early stages of nanomaterials growth also will be offered to users to assist understanding of growth mechanisms, and ultimately to control synthesis.

The Macromolecular and Functional Nanomaterials areas were the two most heavily populated with prospective users at the CNMS' Second Planning Workshop, and parts of each are now in limited operation using existing ORNL facilities in the "jump start" user initiated nanoscience user program.

Nanoscale Magnetism and Transport focuses scientifically on the synthesis and characterization of materials whose characteristic properties and functionalities arise from distinctly nanoscale effects, including the emergence of collective behavior and related effects of reduced and variable dimensionality. CNMS will make available to users a complete suite of scanning probes and unique instruments for nanoscale measurements, described below, to enable studies of the origins of magnetism as well as quantum transport measurements using ultra-thin films, stripes, nanowires, and surfaces.

Research in ***Catalysis and Nano-Building Blocks*** has its focus on the synthesis and characterization of nanostructured catalysts and supports, including studies of nanoparticles/nanocrystals. It will capitalize upon strong synergies with world-class

ORNL capabilities including aberration-corrected atomic-resolution electron microscopy, efficient "compositional spread" catalyst search-and-evaluation methods, and specialized scanning probes, all of which will be made available to nanoscience users. Catalysis is expected to be a rapid-growth area for nanoscale research, and the CNMS user research program will be enhanced by the appointment of an ORNL-U. of Tennessee Distinguished Scientist in this area.

Theory, modeling, simulation and nanomaterials design research will be carried out with users at CNMS through the ***Nanomaterials Theory Institute*** (NTI). The NTI will support users in advancing theoretical and computational nanoscience methodologies that are needed to understand nanoscale materials and phenomena, including addressing computational grand challenges such as the design of functional nanomaterials and virtual synthesis. The NTI also will become a premier Center for the dissemination to users of theory, modeling, and simulation tools that define the computational state-of-the-art for nanomaterials sciences. At the level of facilities and expertise, the NTI will provide nanoscience users with collaborative access to its own staff, postdocs, and visiting Guest Scientists, as well as the full range of facilities and staff expertise at ORNL's *Center for Computational Sciences* (CCS). The CNMS operational budget includes support for CNMS user access to the CCS. On the intellectual level, the NTI will provide a key mechanism for bringing together world leaders and users of computational nanoscience, by sponsoring an international program, tentatively called *User Research Focus Laboratories,* that enables "hands on" development and application of the most powerful techniques to address key issues (of the users' choice) in understanding nanoscale systems and phenomena.

The ***Nanofabrication*** research theme will be carried-out in a new 10,000 sq ft ***Nanofabrication Research Laboratory*** **(NRL)**. The scientific focus in Nanofabrication is on developing new methods for the controlled synthesis and directed assembly of nanomaterials, in order to link nanoscale properties and phenomena up to the microscale and beyond. This research is expected to be strongly coupled with that in Catalysis and Nano-Building Blocks theme area. Methods also will be developed to functionally integrate the use of "soft" and "hard" materials, with a strong scientific focus on nanoscale biomaterials systems, coupling to research in the Macromolecules area. Clean room space and electron beam- and photo- lithography capabilities will provide support for users of all of the other CNMS Scientific Theme areas. The organization and staffing of the NRL's nanoscience user operation is modeled after that of the Cornell Nanofabrication Facility, with additional input from the UC-Berkeley facility (a comparably sized clean room facility). Direct user experience currently is being obtained through operating an interim NRL as part of the ORNL/CNMS "jump start" user nanoscience program.

I.4.b **Unique and State-of-the-Art Instruments and Computational Tools for Nanoscience**

The CNMS' scientific and user-research foci require a balanced approach in selecting its technical equipment set. On the one hand, it is necessary to provide users with high-resolution and high-throughput instruments that often are expensive and therefore appropriate for a user Center where their use can be shared. Despite their expense, these are still "standard" instruments that can be purchased, together with a service/maintenance contract to ensure high-throughput use.

On the other hand, there is a growing need for instruments that provide truly unique combinations of imaging, measurement, and manipulation capabilities, and for corresponding unique and integrative (e.g., multi-scale and for hybrid materials systems) computational tools. Such instruments are available at very few places in the world and usually only as “beta-instruments” that are not generally accessible to users. If they could be made *reliably* accessible to users, their availability would attract forefront science and scientists, and would greatly accelerate discovery and understanding of nanoscale systems and phenomena. In a completely analogous way, there is now an overwhelming need—and a great opportunity because of rapid advances in leadership-class computers—for the development of new computational methods to accelerate understanding complex nanoscale systems and phenomena through modeling and simulation.

The CNMS will support the development and dissemination of new theoretical and computational methods to address nanoscience grand challenges through the *Nanomaterials Theory Institute*.

The CNMS also will provide a home for unique instruments that *define* the state-of-the-art, as well as other state-of-the-art instruments, through the *Nanoscale Imaging, Characterization, and Manipulation* (NICM) Scientific Theme. As has been shown in Table 2, the NICM area is subdivided into three parts to provide expert leadership for development of unique Neutron and X-ray Scattering capabilities for nanoscience; unique new UHV Scanning Probes; and for unique Electron Microscopy and Spectroscopy (SEM- and TEM-based) instruments.

In the following two parts of this section, we list and briefly describe first the truly unique and then other state-of-the-art capabilities that are underway or planned for the CNMS, all with the goal of *reliable user access*.

I.4.b.1 **Unique Instruments and Capabilities that *Define* the State-of-the-Art**

Unique Theoretical and Computational Nanoscience Capabilities (Nanomaterials Theory Institute): Nanoscale Modeling and Simulation Tools and Resources
Extended-period, User Research Focus Laboratories addressing problems of users choice will be utilized within “grand challenge” areas of theoretical and computational nanoscience such as multi-scale modeling; many-body calculations for low-dimensional systems; transport in nanostructured materials; nanomaterials design; virtual synthesis. State-of-the-art tools for modeling and simulation will be developed using the leadership-class, high-performance computers at ORNL’s *Center for Computational Sciences*.

Neutrons for Nanoscience: Unique Neutron Scattering Environments and Techniques
CNMS soon will have access to the world’s best neutron scattering capabilities with the opening of the SNS, and reopening of the upgraded HFIR. Neutron scattering can provide unique information about nanoscale materials and phenomena that is complementary to that obtained by other techniques, particularly for magnetic and “soft” materials systems. Moreover, the pulsed nature of the SNS means that studies of the time evolution of structure and reactions will be possible in such systems for CNMS users. These considerations make it imperative that CNMS provide nanoscience users with easy access to the SNS, by participating in and supporting the creation of special

experimental environments for nanoscience research using neutron scattering. Among the variables that must be controlled are isotopic substitution, temperature, magnetic field, pressure, and fluid flow. A brief list of the special scattering environments and techniques needed includes: (1) high temperature; (2) high pressure; (3) high magnetic field, temperature, and pressure; (4) low temperature and high magnetic field. Development of these will be guided and assisted by workshops with SNS/HFIR and the national neutron scattering community.

Unique UHV Scanning Probes

The "Ultimate STM." Currently under development at ORNL-University of Tennessee, this will be a low-T (300 mK–150 K), high-H (to 9 T) STM for single-atom or –molecule spectroscopy. Atomically-resolved spectroscopy maps and k-space mapping of electronic structure will be made possible through vertical resolution 100X better than commercial instruments. The "Ultimate STM" will provide the range of T, H needed to study the quantum response of nano-objects, together with in-field optical access for probing and exciting atoms or molecules. Other features will include in-field sample rotation, sample exchange from room temperature, and flexibility to convert into a magnetic scanning microscope with atomic resolution.

In-Field SEMPA (SEM with Polarization Analysis). Obtained from the Max-Planck-Institut, Halle, Germany, this spin-polarized SEM provides the 10–15 nm resolution (upgradeable to 3 nm) needed for direct imaging of magnetic domain structures, which is critical for understanding spin reversal and spin dynamics of nanostructures under magnetic field, critical behavior, and spin-dependent transport. This system includes UHV sample environment, sample preparation, UHV electron column, and sensitive spin detection based on spin-polarized LEED. The in-plane 300 mT magnetic field (upgradeable to 800 mT) permits field-dependent studies of domains in deliberately nanostructured materials, with operation at T = 50–1,000 K. Elemental analysis of nanostructures by scanning Auger is a possible upgrade.

Unique Electron Microscopy and Spectroscopy Capabilities

Nanomanipulator and Probe for TEM. Planned for development is a dual-probe device that can mechanically, electrically, magnetically, or thermally interact with samples in a TEM. This device is essential for nanomaterials research, permitting conductivity measurements of individual CNTs or other nanoscale features; controlled loading and displacement to determine strength, elastic moduli or other responses; and localized heating or cooling to intiate reactions and modify properties. This probe will be more complex but also multifunctional, compared with prototypes.

Field Emission Gun (FEG)-TEM for Holography/Tomography. Available on existing microscopes at ORNL and the University of Tennessee, holography permits imaging at high resolution and high contrast materials that have little inherent contrast in conventional microscopes (CNTs, composites, polymers, protein complexes), as well as direct visualization of electric and magnetic fields. Used with the planned addition of a Nanomanipulator/Probe, the FEG-TEM will permit measuring piezoelectric responses to mechanical displacement, or magnetic responses to a magnetic probe. It will be possible to visualize magnetic and electric field distributions in 3D through combined holography / tomography.

Aberration-Corrected SEM / in situ AFM / Probe + Micromanipulator System. In this planned system, with aberration correction, the sample can be positioned more than one centimeter from the electron lens without loss of resolution. This provides space for the AFM and manipulator package as well as sample tilting, so that the same area is viewed in both the SEM and AFM images. This system will be able to image materials that cannot be prepared suitably for TEM. Simultaneous correlative SEM/AFM imaging will remove imaging ambiguities, and the wide range of topographic, chemical, and electronic information generated by the SEM using secondary and backscattered electrons, fluorescent x-rays, and cathode-luminescence can be combined with the 3D surface imaging. The similar spatial resolutions of the two imaging systems (due to aberration correction) result in highly specific characterization, including a "nano-metrology" capability to verify results from the nanofabrication facility, down to the resolution limit of the e-beam writer. *A truly world-class instrument*.

I.4.b.2 **State-of-the-Art Nano-Characterization Tools**

<u>Time-Resolved, *in situ* Spectroscopic Diagnostics</u>. A unique and powerful combination of fast, time-resolved *in situ* optical imaging and spectroscopic diagnostic techniques will be made available to users, to assist understanding nanomaterials growth mechanisms in laser vaporization and chemical vapor deposition growth systems. The methods include fast intensified CCD-array (ICCD) imaging; blackbody emission spectroscopy and laser-induced incandescence (LII) imaging for thermometry of hot ejected particulates; optical absorption and emission spectroscopies (OAS/OES) and ion probe analysis, to identify and understand multi-component fluxes during nanomaterials growth; laser-induced fluorescence (LIF) studies of molecules formed in gas-phase collisions; Rayleigh scattering imaging of small nanoparticulates and aggregates as they form; gas-phase photoluminescence spectroscopy (PL) and imaging of nanoparticles having high transient brilliance; and Raman spectroscopy to probe nanotube or other nanorod/nanowire growth.

<u>Nanomaterials Optical Characterization Facility</u>. Raman spectroscopy, fluorescence, and photoemission are examples of optical spectroscopy techniques that are essential for the rapid, remote, nondestructive assessment of crystalline structure, defects, and electronic energy levels in nanoparticles, nanorods, polymers, and carbon nanotubes. A state-of-the-art but user-friendly system comprised of a tunable laser, microscope, and high-resolution monochromator will be available for use in probing the optical properties of functionalized nanomaterials synthesized at CNMS. An all solid-state, tunable laser system will provide low-energy, picosecond pulses at high repetition rate with sufficient average power and narrow bandwidth for resonant Raman spectroscopy and other measurements of carbon nanotubes and other nanomaterials, across the entire UV, visible, and near-IR regions of the spectrum. The tunable laser will be coupled to a high-resolution monochromator and optical microscope for unprecedented optical investigations of micron-sized regions of samples.

<u>Four-Point-Probe STM with SEM</u>. Commercially available, this instrument enables temperature-dependent quantum transport measurements of nanoscale objects on surfaces: spintronics, spin injection, spin transport. It combines accurate four-point measurements of electrical transport with nanoscale STM sensitivity. The integrated SEM with < 10 nm resolution allows accurate, independent positioning of all four tips with separations < 100 nm. One probe can be used to fabricate a feature by STM-induced CVD, followed by direct imaging of the fabricated nanofeature by another tip, and accurate four-point transport properties measurements around the feature. Operation at T = 20–600 K and UHV-capable.

Nano-Transport Synthesis and Characterization System. This system will be used for growth, characterization, and in-situ electrical transport studies of low-dimensional transition metal oxide (TMO) structures. Four UHV vacuum chambers are connected through a central chamber for sample transfer under vacuum. The first "laser MBE" chamber combines conventional MBE sources with pulsed excimer laser ablation and differentially pumped RHEED, and is the best approach for controlled growth of crystalline TMO films. The second chamber is dedicated to electron spectroscopies (XPS, AES, and LEED for surface analysis) and to macroscopic transport measurements between 20–400 K using a four-point probe. The system also will be equipped with MOKE to identify magnetic properties. A third chamber will house a variable-temperature SPM that functions as an STM for atomic-resolution structure and as an AFM capable of nanometer-resolution transport studies. Electrical transport across individual defects, grain boundaries, and phase separation regions can be determined by mapping both ac and dc potentials. A fourth chamber will be added for HREELS, to identify surface species through vibrational analysis and to distinguish electronic states through low-level excitations.

Instrument Suites for Nano-Characterization (CNMS ground-floor labs and clean room)

Scanning Probes Suite: Spatially resolved characterization of atoms, spin, and charge. Electronic structure (STM), topography (AFM), magnetization (MFM), transport, piezoresponse FM, potential mapping.

Electron Microscopes Suite: SEM/FIB for sample preparation; metrology SEM; conventional TEM/STEM imaging (initially this capability will be located at the main ORNL site); SEM for chemical analysis (EDX); all located in electromagnetically, vibrationally, and acoustically shielded laboratories at the east end of the *Nanofabrication Research Laboratory*.

I.5 **Management Plan**

I.5.a Scope of Operations

The scope of CNMS operations includes:
- Operate laboratories and offices with high reliability and safety and in compliance with regulations
- Manage a highly collaborative and world-class nanoscience user research program of approximately 250 users and 7,500 user-days in FY2008
- Operate and provide support for an appropriate concentration of unique and/or state-of-the-art instruments and expertise so that users have reliable access to both
- Continuously improve the operation of key instruments and capabilities
- Together with the national user community, carry out R&D and make the additional investments needed to keep the CNMS at the instrumentation and computational "frontiers" that define state-of-the art nanoscience capabilities
- With input from advisory groups and the user community, periodically redirect the CNMS' effort to focus on the most important scientific opportunities

In brief, the goal is to manage the CNMS so as both to operate a world-class and a highly reliable user research facility and simultaneously to refresh and enhance its capabilities

I.5.b CNMS Management and Administration

Figure 1 (section I.3) shows the proposed organization of the CNMS. The CNMS will be led by Doug Lowndes (Director) and Linda Horton (Deputy Director). From its conception, CNMS has had a strong, multidisciplinary scientific leadership team made up of the key scientific leaders for the scientific thrusts of the CNMS. With initial user operations, Tony Haynes has joined the team as the User Coordinator. In operation, this team will be further expanded to include operational staff for the laboratories in the CNMS. In the following section, the responsibilities for the various offices and activities for the CNMS are briefly summarized.

Director's Office. The Director's Office has primary responsibility for the successful operation of the CNMS and has line responsibility for staffing, budget, and support functions, including environment, safety and health. It ensures integration of the CNMS with the balance of ORNL's facilities. The Director's office administers the CNMS Guest Scientist Program and the CNMS Postdoctoral Scholars program. The Director's Office includes one clerical/web support person, 2 clerical support personnel for the DD and CNMS staff, and 2 ESH support people (one located in the SNS building), and 0.5 financial support person (located with SNS).

Working with the CNMS scientific leadership, the Director has primary responsibility for developing a world-class user and in-house nanoscience research program, and for initiating actions to continually improve it. The Director leads external outreach and interaction activities, both those focused on the CNMS (SAC, PRC, and UEC) and those involving other DOE- or university-based nanoscience research Centers. The Director also administers and approves any user proposals requesting rapid access to the CNMS (see section I.6).

The Deputy Director has primary responsibility for the facilities, equipment, and operation of the CNMS, including oversight of user support functions. In addition, the Deputy Director is responsible for integration of CNMS within ORNL, including the relations with SNS and other ORNL user facilities.

User Coordinator's Office and Support: This Office is responsible for administering the user program. It will issue calls for proposals, coordinate the review processes, and coordinate the scheduling of the selected research projects, including all required paperwork and user agreements. The current proposal review process is outlined in Figure 2. Information required for user reports, statistics, user feedback, etc., also will be gathered by this Office. This Office also will coordinate the development of required web-based user training and instruction modules. Many of the functions of this Office will be augmented by the SNS user support group. Close integration between these two offices will be critical to ensure that CNMS develops an outstanding reputation with users. In addition to the User Coordinator, this Office includes 1.5 user-support personnel, one located with CNMS and 0.5 with SNS.

Scientific and Operational Leadership: Operational Leaders who will be responsible for reliable, safe operation of the CNMS laboratories and for the success and quality of the user research experiences have been identified for each of the Scientific Theme areas (boldfaced names, Table 2). This group has the equivalent of line management responsibility for CNMS activities. Scientific Leaders, also identified for each of the scientific themes, are responsible for ensuring the quality of the science, scientific direction, and the vitality of the user community. Together, the operational and scientific leadership make up the backbone of the CNMS user program. These leaders together with the Director, Deputy Director, and User Coordinator, will make up the CNMS.

Leadership Team. Regularly scheduled meetings of this group will be held to ensure optimum operation of the CNMS and integration of the user program.

The CNMS Leadership Team will be a natural extension of the current CNMS Project Scientific Leadership Team, most of whose members have been working together on the CNMS project since before the original CNMS proposal was submitted to BES. During the evolution of the project, additional members were added to the original team to meet scientific needs (e.g., leadership for the *Imaging, Characterization, and Manipulation* area) and when the user nanoscience program was initiated (the User Coordinator). It is expected that the CNMS Leadership Team will evolve in much the same way. While the current group meets monthly, it is anticipated that more frequent meetings will be required during the first months of operation in the new facility, probably twice monthly.

Laboratory Space Managers. In January 2004, ORNL implemented a Laboratory Space Manager program to more effectively manage laboratory space and activities. CNMS laboratories will be administered under this program. Each laboratory in the CNMS will have a designated Laboratory Space Manager who acts on behalf of the Operational Leader to oversee activities in that laboratory. The Laboratory Space Manager acts on behalf of the Operational Leader as a steward of the assigned laboratory space, providing in-lab knowledge and guidance for both users and staff to ensure reliable, safe, orderly, and compliant operations.

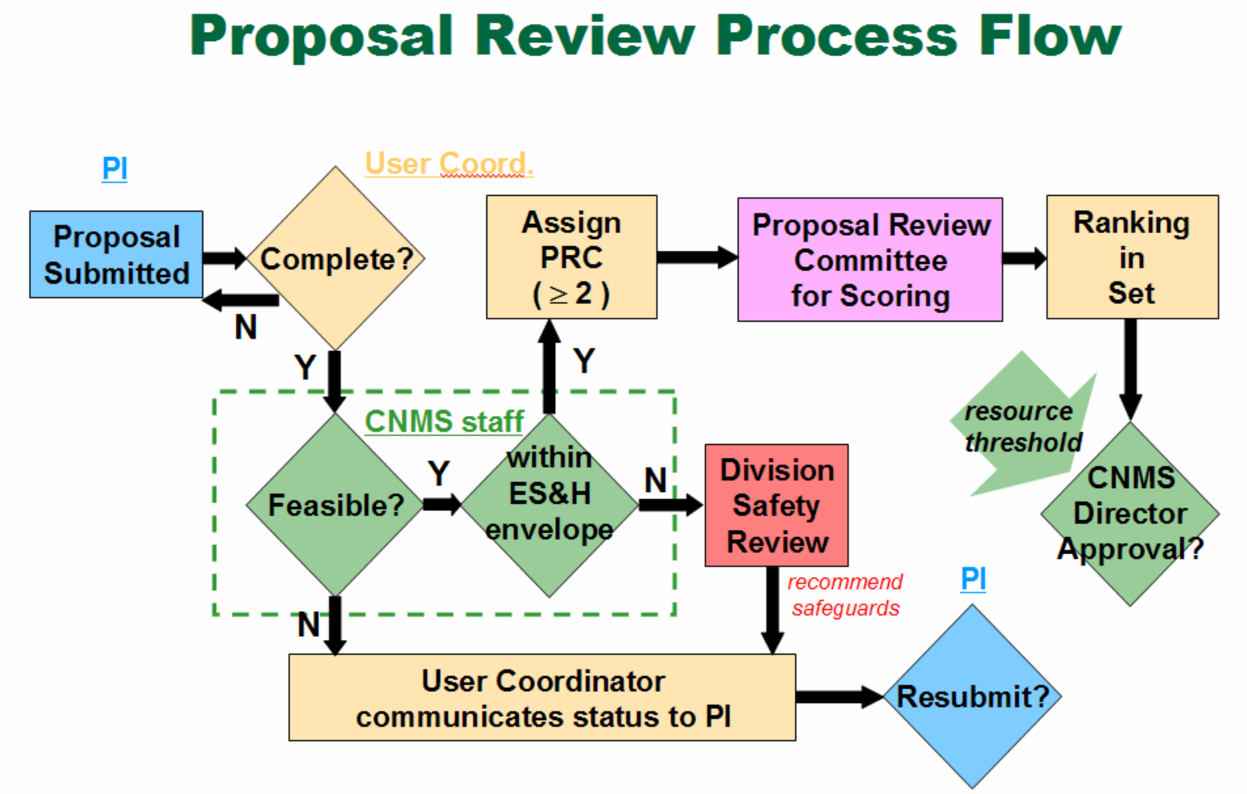


Figure 2. Proposal review process for CNMS user proposals.

I.6 <u>User Policy and User Modes</u>

In order to be responsive to user needs while also providing flexibility for development of unique new capabilities through user collaborations carried out at the CNMS, the CNMS user program will support two modes of user access, General User and Partner User, both of which are defined in the "General Policies and Procedures for User Access to the DOE Nanoscale Science Research Centers" (see Appendix C).

<u>General User</u>. The category of General User permits routine access to the facility to use existing CNMS equipment for the conduct of user research. The vast majority of users will enter CNMS through the General User mode. The scope of General User projects may range from a single experiment, involving a relatively small equipment set and one or two visits to the facility, to research program-level proposals that extend over many visits, require access to a wide range of equipment and may continue for multiple years based on successfully reviewed renewal proposals. This category may also include collaborative proposals that involve CNMS staff members as principals in the scientific team.

<u>Partner User</u>. The CNMS must remain at the forefront in developing novel techniques and instrumentation in order to maximize the facility's benefit to the nanoscience user community. The Partner User mode of access is designed to encourage significant research collaborations that also enhance the capabilities or contribute to the operation of the CNMS. The outcomes of Partner User proposals are new or enhanced capabilities that must be made available to the General Users and so benefit them as well as the facility. Partner scientific programs are subject to the same peer review process as General Users. As part of that review process, Partner User proposals at the CNMS are evaluated by external reviewers on the additional criterion of the anticipated benefit to the CNMS user community. Partner Users may be allocated limited access to one or more facilities that are needed to accomplish their research objectives over a period of several years, with the possibility of renewal.

When a new capability is being developed, for example by an identified Instrument Development Team (IDT), this period may include a transition period from exclusive use by the Partner User during the initial development phase (no CNMS support provided for use by General Users), through a “beta-phase” involving selected “friendly” users (limited support for General Users), before becoming part of the general access capabilities with full user support provided by the CNMS. Periodic peer reviews of progress will be conducted throughout the development period in order to determine when the reliability and value of the new capability have become sufficient to justify full availability and support as part of the CNMS user program. Partner projects normally will be expected to reach such a level of maturity within a predetermined time or be subject to cancellation, as determined by the peer review.

Proposal Submission Cycle. Normally, proposals will be accepted on a periodic cycle, with frequency determined by user demand and in consultation with the Users’ Executive Committee. This cycle will likely be adjusted to be commensurate with the scheduling cycle for other major user facilities at ORNL in order to facilitate coordination of user access to those facilities.

Rapid Access. The CNMS also will support a small number of rapid-access proposals that may be submitted “off cycle” within the General User category. Rapid-access proposals may be approved at any time at the discretion of the CNMS Director. The CNMS Director may request an expedited peer review of each rapid-access proposal in order to advise his/her decision on a case-by-case basis. The rapid-access proposal process is necessary to provide an avenue for rapid decisions on proof-of-concept (feasibility) studies that involve only small amounts of CNMS resources but are particularly time-sensitive. A successful rapid-access project would normally be expected to lead to a standard user proposal submission in the next scheduled cycle.

Proprietary and Non-Proprietary Research. The vast majority of user research should be in the public domain and so must be disseminated by publication in the open literature. However, the NSRC “General Policies and Procedures” permit access for proprietary research that utilizes these unique facilities *to benefit the national economy*. Users conducting such proprietary research may access the facility as either General Users or as Partners. Full cost recovery will be obtained for such proprietary research, and efforts will be made to secure appropriate intellectual property control for proprietary users to permit them to exploit their results.

II. Staffing and Budget: GUIDING PRINCIPLES AND ASSUMPTIONS

II.1 <u>Integrative Nature of Nanoscience and Consequences</u>

Nanoscale science is highly integrative of knowledge and disciplines. Consequently, a user normally will need capabilities that are found in more than one of the CNMS' Scientific Theme areas. Examples might include work in *Macromolecular Complex Systems* (for polymer synthesis) and *Nanofabrication* (for soft-hard materials integration in a structure); or research in *Nanoscale Magnetism* (for synthesis) and *Nanoscale Imaging and Characterization* (to use the SEMPA); or work in *Functional Nanomaterials* (for nanowire synthesis) and *Nanoscale Imaging and Characterization* (for quantitative chemical analysis and quantum transport measurements). Thus, it should be expected that there will be a need to optimize the staffing of different Scientific Theme areas with respect to each other, as operational experience is gained and specific user needs are determined. However, this "fine tuning," while changing the details of who is supported at what level, should not have significant impacts on the budget for the overall staffing for CNMS.

This document is based on

(1) the current estimated requirements for operation of the individual Scientific Theme areas based on actual research experience in similar areas at ORNL and benchmarking discussions with other institutions, especially for the cleanroom operations;
(2) anticipated interactions and synergies among these areas, e.g., the development of unique instruments to enable specific types of research; and
(3) preliminary knowledge of user proposals and the resulting staffing requirements that was obtained in evaluating the first round of proposals in the FY2003–4 "jump start" of user-initiated nanoscience research at ORNL.

II.2 <u>Sources of Funding</u>

BES/DOE is expected to provide the operating funds for the CNMS. This staffing and budget plan assumes an initial operating budget of $18.5M in FY2006, the first full year of CNMS operation, and increments of $500K/year for FY2007 and FY2008. It is significant to note that this level of increase *will not cover* a 3% escalation of costs. At BES' request, our plan also considers what important new/additional user nanoscience research could be accomplished if 10% additional budget was added to the $18.5M base.

DOE and other funding agencies also may provide significant equipment upgrades, or additional equipment, instruments, or facilities, e.g., in response to collaborative proposals for advanced instrumentation. The operating funds identified in this budget support the reliable delivery of nanoscience research capabilities to users, with the level and variety of capabilities determined both by user demand (expressed in user proposals and CNMS-sponsored planning workshops) and by the available DOE funding. At CNMS, the projected operating budget will support minimal incremental upgrades and will provide very limited support for major instrument investments, in order to make *unique* instruments that *define* the state-of-the-art in nanoscale imaging and characterization available to the user community. However, neither the operating budget nor the CNMS' staff scientists' intellectual resources alone are expected to be sufficient to achieve the latter ambitious goal. To ensure that the CNMS' research capabilities remain close to the "instrumentation frontier" and are responsive to cutting-edge scientific needs of users, planning workshops, focused symposia at national meetings, and development of collaborative teams for instrument development proposals will be employed. In addition, long-term Guest Scientist positions have been incorporated into the staffing plan (a SAC Recommendation) in order to bring in the best scientists and ideas from around the world to work with CNMS staff to develop instruments that will *define* the state-of-the-art. Collaborations among users may result in the development of proposals for major advances in instrumentation, for submission to DOE as well as other funding agencies. CNMS will be responsible for the staffing/operational/maintenance support needed to ensure *early and reliable access* by users to what otherwise might be only "beta-tools" for nanoscience, accessible to only a few.

In addition, it will be necessary to request that DOE-BES provide the equivalent of "Accelerator Improvement Project" (AIP) funding beginning in FY 2009 to upgrade major user instrumentation. Assuming a 5-year technology lifetime for the leading instrumentation, the budget needs in this category will far exceed what can be accomplished with normal capital funding resources. The funding needed in this category is estimated to be $3M per year, with occasional increases to the $5 to 6M level to upgrade single instruments in this cost range.

II.3 <u>User Access</u>

The operational goal for user access to the CNMS will vary over its seven Scientific Theme areas. The initial operation goal is 12hrs/5 days availability of equipment for *hands-on* operation, with the option of 12 hrs/6 day operation of the clean room and other high-demand equipment. Not included in these operation hours are normal overnight activities such as standby or preparative operations (e.g. pre-baking or pump down of a synthesis system or characterization instrument) and overnight computer runs. In this type of user operation, interaction time is often the limiting factor in available user time. So, one of the major considerations is available staff time to work with users. After extensive training, many users will be able to use much of CNMS instrumentation without constant oversight. However, the presence of technical support and ESH staff in the vicinity will be critical to insure the safety of the users, protection of the environment, or the proper use of the instrumentation itself, for many (though not all) types of research activities.

II.4 <u>Reliability of Operation and User Metrics</u>

In considering metrics for a nanoscience user operation, it is important to recognize that the integrative nature of nanoscale research requires simultaneous parallel staffing of Scientific Theme areas that utilize quite different expertise. This is fundamentally different from operating a "beam" facility, in which a single set of research staff/technicians can make the beam simultaneously available to a multitude of users with diverse backgrounds, but with each user group providing the diversity of experience that is needed to support its own research. Thus, to make the CNMS' operation effective for nanoscience users will require taking as high priorities:

(1) carefully integrated scheduling of users;
(2) instrumentation that is best of class and designed/staffed to facilitate user operations; and
(3) highly reliable operation of the individual instruments/facilities.

These are ambitious goals that require readily available spares, service contracts and access to well-trained instrumentation technicians, and dedicated operations staff; regularly scheduled upkeep and maintenance of materials synthesis and characterization facilities and instruments; and, ready access to support shops and facilities. As noted in discussions of the operation of major beam facilities, users want—more than anything else—reliable, predictable research support.

In view of these considerations—particularly the likely use of more than one Scientific Theme area by a user within a single day or visit—the most appropriate metrics for NSRC operation seem to be (1) number of users (a common metric for user facilities); (2) both the numbers of repeat users (indicating quality experiences and good collaborations) and of new users (indicating a growing community and openness of access); (3) user-days; and (4) resulting publications. The latter should be considered both in the best of journals and in discipline-specific publications that reach all of the scientific community.

Considering first the number of users, the CNMS operational goal will be 100 users during FY06, 200 users in FY07, and 250 users in FY08. With the budgeted staff, CNMS has a goal of reliably providing 10,000 user days of support to the community per year once it is in steady state operation. Due to the nature of synthesis and computational research, in particular, "days of user support" includes both the actual days that a user is onsite and the additional days during which the synthesis/calculations that began during an on-site visit may be ongoing and consuming the full-time effort of a CNMS staff member or postdoc, with the user at his/her home institution. In both the actual proposal for the user project and in the assessment of CNMS performance, this time must be counted as a "user day" since these activities require both staff and equipment time; i.e., this time will not be available for other user projects. The goal for FY06 is to provide 2,000 user days of support, with growth to 5,000 by the end of FY07, and 7,500 user days in FY08. The reason for this progression is that there will be more need for equipment optimization, training, preparation and testing of web-based learning modules, and other developmental activities during the first years of operation of the CNMS. Thus, the goal is to increase both the number of users and the quality of the user research support and collaboration as the program matures. For the BES Shared Equipment (SHaRE) User Program at ORNL (a mature user program that focuses on analytical electron microscopes) the average number of user days per user is between 20 and 25. Given the additional user days required for synthesis and computational research, we anticipate that this metric may exceed 30 days for the CNMS.

The number of user-days provided per year can be related directly to the size of the CNMS staff and the fraction of time that each employee spends working with users. The 10,000-user day goal assumes that employee scientific staff will work directly with users for 65% of the time that they charge to CNMS, technicians for 80%, and postdoctoral staff and visitors for 50% of the time that CNMS supports. The balance of the time for the employee scientific staff will be divided between personal research (15%) and equipment development/maintenance (20%). The balance of time for technicians will be devoted to equipment maintenance/development. For postdoctoral staff, the balance of the time supported will largely be devoted to development of their research skills (likely largely focused on development of new instrumentation and techniques for nanoscience that also will benefit users). The purpose of the Guest

Scientist positions is to bring in unique expertise, so the remainder of their support will be the development of new instrumentation and research techniques for the national user community.

II.5 **CNMS Site, ORNL Infrastructure Support, and Basis for Cost Estimates**

The CNMS will operate under ORNL business and financial rules, and within the ORNL Physical Sciences Directorate. The CNMS will be a multidisciplinary Center. With the addition of shared research staff and estimated daily user population, the total staff in the building on a daily basis will easily exceed 150, with maximum available office space (including quad-office arrangements for graduate students, short term visitors, and technicians) for 190.

The operational budgets for FY2006–8 have been planned using the current organizational structure represented by Figure 1 and Table 2. The detailed organization of Scientific Themes and Research Focus Areas may change as the CNMS project moves from construction to operations. Also, as noted elsewhere, Research Focus Areas will evolve, in order to address the most important and timely scientific challenges and technological opportunities, and keep CNMS focused on the highest priorities. However, the functions represented in the budget are expected to appear in any similar research areas for CNMS, so the overall budget should not be affected in any dramatic way by changes in relative priorities.

The balance of this section provides the foundation used in the development of the budget estimates. Additional details are provided in section III, the detailed staffing plan and budget.

Infrastructure Support: Maintenance and upkeep of the CNMS building infrastructure will be supported through the ORNL space charge-back program, which also will maintain the adjacent SNS Central Laboratory and Office (CLO) building. Maintenance, upgrading, and replacement of all CNMS research instruments and technical equipment will be supported directly from operating funds, capital equipment funds, and, in the longer view, AIP funds as discussed above.

Utilities at ORNL are also charged at a per square foot rate. For this budget, it is assumed that CNMS utilities will be part of this assessment. This is the requirement for other new buildings recently occupied at ORNL. Other elements of infrastructure support include telecommunications and information technology access charges. These are included and charged at the expected ORNL rate for these services.

Shared Infrastructure and Support - Integration with SNS: The CNMS is located on ORNL's SNS "new campus." Therefore, a large part of the CNMS infrastructure is supported by site utilities that are shared with SNS. Shared facilities include the boiler, chillers, electrical substation, and the alarm system (which will be routed to the SNS control room in addition to sounding locally). An Operational Agreement is being executed between CNMS and SNS to document shared staffing for ESH, user support, information technology, procurement, building support services, and technical support (specialized instrumentation technicians, for example). Longer term access will be negotiated for the user machine shops, stock rooms, etc. CNMS users and staff also will have access to the SNS "public" facilities (cafeteria, library, conference rooms, etc.)

CNMS clearly benefits financially from the considerable economies of scale and more efficient use of space that result from these infrastructure arrangements with SNS.

Note: At ORNL general infrastructure support as well as general administration and ESH support are typically gathered and charged to programs as part of an hourly rate for staff-time that is called “organizational burden.” For simplicity at this stage of budget development, these costs are detailed individually in the budget documentation. In final operations, these costs may be distributed through an organization burden model, but the cost to the program will be the same.

Technical Support: Services will be provided to users to support world-class research. Technical and support staff will enable users of varying experience levels to carry out their research programs. As discussed above, basic administration, user, ESH, and related services will include shared staff with the SNS. For operational efficiency, there will be dedicated user administration and ESH expertise in the CNMS. The budget for technical support staff for daily user R&D has been developed by the operation and scientific leadership of the Center. Current levels allow for about 1 technician for every 4 labs in the main part of the building, with additional specialized staff for computer support, instrumentation, etc. The Nanofabrication Research Lab clean room is a special laboratory for which the staffing levels were developed after consulting with similar clean room R&D operations, notably the Cornell Nanofabrication Facility. There are currently 8 technicians assigned to the clean room with the understanding that *extending operations will result in the need for additional staff, both technical and ESH*.

R&D Maintenance Activities: Maintenance of research equipment and related R&D activities for CNMS will be provided through subcontracts or through support of appropriate ORNL staff. Crafts personnel and associated machine shops will be available on both ORNL campuses. Maintenance and refurbishment budget estimates are assumed to be a percentage of the staff costs for each of the Scientific Theme areas. Since staffing levels are roughly correlated with numbers of instruments operated for the users, this approximation has proven to be reasonable. The upper end of the budgeted amount (20%) is applied to the clean room and electron microscope facilities, i.e. to equipment with expensive service contracts. The lower end of the budgeted amounts (1%) is for the office-based activities, including the theory efforts. The majority of the Theme areas are budgeted at 5% of staff costs. These estimates have been validated based on combined ORNL experience with (1) the cost of service/maintenance contracts for major instruments (e.g., electron microscopes) in user facilities (e.g., SHaRE, HTML); (2) service/maintenance contracts for smaller laboratory instrumentation; and (3) staff scientists’ estimates for other maintenance and refurbishment costs.

Waste: Wastes will be handled by the ORNL Waste Management organization, based on the *ORNL Waste Management Plan*, with waste disposal costs borne by the activity generating the material and funded by the operating budget. In the CNMS budget, the cost for this service is included in the “maintenance” budget category for each theme area, with non-task specific costs included as part of the building miscellaneous budget. Experience with similar organizations at ORNL suggests that the total cost of this activity will translate to 0.25 to 0.5 FTEs, or less than $100K (before overhead) for the entire facility.

Travel: Travel budgets have been estimated at 3% of the scientific staff cost. This methodology parallels that used by the Spallation Neutron Source. An alternate approach considered was to assume a fixed budget/number of trips per FTE supported. An assessment with this alternate approach supported the budgets determined by the method used. The average travel budget per scientific FTE is roughly $4,000 with some variations by scientific theme.

Consumable Materials (including spares): Materials requirements have been considered in detail by Scientific Theme area leaders, but the basic budgets were again based on staff costs since research costs and materials are largely correlated with the staff required to perform/operate the research/instrumentation. The percentages used in the budget calculation ranged from 3% for the administration offices to 20% for the clean room and microscope facilities. For most of the research, the assumption was 10%.

Note that shipping and receiving for the SNS site will be handled as part of an existing ORNL organization. The costs for this are incorporated in the materials overhead charges. There are easily accessible loading docks both at CNMS and in the SNS CLO for deliveries of materials.

Proprietary Research: Although most research at the CNMS will be made available publicly, proprietary research will be possible under special arrangement and at rates commensurate with ORNL and DOE policies (see section I.6 and Appendix C).

II.6 <u>**CNMS Staffing Levels and Shared Staff**</u>

Estimates of needed operating staff levels are based primarily on a bottoms-up evaluation of the tasks involved. When possible, the staff levels are compared directly with corresponding ORNL activities and those of other ORNL User Facilities. For several of the Scientific Theme areas, a second basis for estimation is the research staff and postdoctoral staff needed to support users in ORNL's new "jump start" user-initiated nanoscience research program (a precursor to operation of CNMS).

Especially in these initial years of operation, the CNMS will make significant use of shared research staff in order to provide users with the level and type of nationally leading nanoscience expertise that is the basis for ORNL operating an NSRC. The affiliations of such shared staff with both CNMS and their ORNL division will be clearly shown on each staff member's CNMS web page. This provides the added benefit that nanoscience users will be made aware through this linkage of related research activities and programs at ORNL. From a cost perspective, although shared staff also will have an ORNL division affiliation, none of the home division's overhead costs will be charged to CNMS for research done in the CNMS building. This condition has been agreed to by the participating divisions and is supported by Jim Roberto, the Associate Laboratory Director responsible for both CNMS and the line physical sciences research divisions. Clearly, for services and activities that take place in the laboratories supported by another organization the costs associated with these laboratories will have to be paid for by CNMS following the standard charge-out process.

The guiding principle to determine cost-sharing for NSRC staff is that there should be *equity for both the CNMS and the other ORNL program(s), i.e. that both should benefit from sharing staff*. To ensure that cost-sharing of staff members is appropriate from the perspectives of both CNMS and other Laboratory units, as discussed earlier, CNMS has established a Management Integration Team consisting of the leadership of all of the affected Laboratory divisions and DOE programs (see Table 1, section I.3).

III. DETAILED STAFFING PLAN AND DETAILED BUDGET

III.1 CNMS Staffing

The CNMS will include a diversity of staff to meet the needs of the user community. Table 4 below summarizes the staffing mix and the associated budget requirements (including fringe, excluding ORNL overheads). The core scientific staff consists of 26 full-time-equivalents (FTEs) with a mix of senior scientific leaders and junior staff. The number of ORNL scientific staff to be housed at the CNMS is nearly 50.

The actual staff (projected at this time, some are TBD) and associated percentage of time to be spent on CNMS user activities is shown in Table 5 on the next page. About half of these represent new hires: about 18 of the scientific staff, much of the user/administrative support staff, and nearly half of the support staff. We have already hired part of these staff as part of the initial user activities, and others are planned from the ranks of existing postdoctoral staff. In addition, we have identified several positions for critical or general hires (staff for whom ORNL pays part of the initial year salary to help develop new programs as part of the Laboratory Director's Research and Development Program).

Of the scientific staff, 14 are full-time CNMS staff, an additional 11 have 50% or more support, and an additional 18 have 20% or greater support. The staff with less than 20% support fall into 2 groups: Staff whose expertise is needed on a limited basis for specific techniques and senior scientific leaders who will do extensive outreach with the technical community, work with users on a limited basis, and will provide scientific leadership for postdocs and younger staff members.

Coupled with the senior staff will be a small population of guest researchers who will bring complementary expertise to the CNMS in nanoscience synthesis, development of equipment, and characterization. We expect that most of this group will be university staff on sabbatical research who will receive about 50% of their support from CNMS, resulting in a total of about 18 people (9 FTE supported). In addition, there will be 25 FTEs of postdocs. The postdoctoral population will largely be only partially supported by CNMS, with the balance of their support from collaborative programs at ORNL and at partner institutions. We estimate that the actual postdoctoral population at CNMS will approach 40 at any given time.

Critical to the success of the CNMS are technical and user support staff. CNMS will support about 17 FTEs of technicians. The majority of the technicians will be dedicated to CNMS user activities. While the majority of the 5 administrative support staff will also be dedicated to CNMS, at least 1 of the user support staff will be shared with the SNS. Likewise, while at least 1 full time ESH staff member will be located in CNMS, the balance of the ESH staff will be shared with SNS or other ORNL organizations to insure the required diversity in technical expertise.

Later in this section of the documentation are individual sections that detail the staffing for the administrative/management and for each of the scientific themes.

Table 4: Summary of Staff FTEs and Cost (without overhead)

Cost Summary		Sci FTEs	Support FTEs	Postdoc FTEs	Guest FTEs	Staff Cost
	FY2006	26.4	24.0	25.0	9.0	8,317,682
	FY2007	26.7	24.0	25.0	9.0	8,628,287
	FY2008	26.7	24.0	25.0	9.0	8,905,533

CNMS Staffing (continued)

Table 5: CNMS Staff with Percentage Support

Management
Lowndes, Doug (1.0)
Horton, Linda (0.5) – incr to 0.75 in FY 07
Haynes, Tony (1.0)

Scientific and Operations Leaders
Anderson, Ian M. (0.3)
Baddorf, Art (1.0)
Britt, Phil (0.6)
Christen, Hans (0.5)
Cummings, Peter (0.25)
Egami, Takeshi (0.2)
Geohegan, Dave (0.5)
Joy, David (0.25)
Kasica, Rich (1.0)
Larson/Ice - affiliated
Overbury, Steve (0.2)
Plummer, Ward (0.3)
Schwartz, Viviane (1.0) – **New hire**
Shen, Jian (0.3)
Simonson, Mike (0.2)
Simpson, Mike (0.3)
TBD, Dist Sci catalysis (0.2)
New hire
Wendelken, John (0.5)

FTE Support Staff
Administrative/ User Support (5)
- **3 new hires**

Technical Support (17)
- **8 new hires**

ES&H (2)

Guest Research Staff
Postdoctoral Fellows (25)
Guests (9)

Balance of Research Staff
Dagotto, Elbio (UT Dist Sci **new hire**) (0.1)
Doktycz, Mitch (0.1)
Hong, K. (1.0) – **new hire**
Kalinin, Sergei (0.4)
Mays, Jimmy (0.1)
Schulthess, Thomas (0.2)
Stocks, Malcolm (0.1)
Varela, Maria (0.25)
TBD (1.0) (bio/polymers) **– new hire**
TBD (0.6) (bio/polymers) **– new hire**
TBD or Alex Puretzky (1.0) **– new hire**
TBD or Ilia Ivanov (0.5) **– new hire**
TBD or Zhengwei Pan (0.75) **– new hire**
TBD or Chris Rouleau (0.3)
TBD or Zheng Gai (1.0) **– new hire**
TBD or An-Ping Li (1.0) **– new hire**
TBD, catalysis (1.0) **– new hire**
TBD, UT Dist Sci new hire, theory (0.1) **– new hire**
TBD, Theory (1.0) **– new hire**
TBD, Theory (0.75) **– new hire**
TBD, Theory – RFA support (1.25, 5 @ 0.25)
TBD or X. Zhang (0.5)
TBD, clean room (2.0) **– new hires**
TBD or Minghu Pan (0.75) **– new hire**

Staff with 100% CNMS Support
Staff with 50% or greater support
Staff with 20% or greater support

III.2 Operating and Capital Budgets: FY 2006, 2007, and 2008

The projected Operating Budgets for each of the fiscal years are summarized in Table 6 below. The details of these budgets can be found in the individual sections for each scientific theme later in this documentation.

The overhead rates for ORNL and other relevant rate information are listed in Table 7. Note that the DOE quoted escalations are less than the escalation rates for salaries and utilities used in these estimates. The assumptions are based on current budget guidance from ORNL.

Details on Budget Calculations: This section will describe the basis for the cost estimates. Note that ORNL charges different overhead rates on different types of costs.

Staff Cost: FY06 salary costs for employees are based on the ORNL quoted wage pool hourly rates for different types of employees. These rates include an average hourly wage for similar employees plus the fringe costs and a small amount of overhead associated with managing the salary/fringe pools. ORNL assumes that a full year is 1800 working hours for all staff. Escalation for out-years was at 3%. In the calculation of overhead costs on employee salaries, G&A is charged against the salary cost; the Award fee percentage is paid on both the salary cost and on the associated G&A.

ORNL postdoctoral staff are actually employees of Oak Ridge Associated Universities, a separate DOE contractor who manages ORNL's postdoc program. The annual per year cost includes fringe and overhead charged by ORAU for managing the program. Note that ORNL charges no additional overhead on postdocs. The FY06 postdoctoral rate represents a broad average for postdoctoral fellows in the various disciplines that will be represented at the CNMS. Escalation for out-years was also at 3%.

Table 6: Summary of Operating Budget by FY

Summary	Staff Cost	Travel	Maintain.	Consumables/Materials	Building Support	ORNL OHs/Use Tax	Total Operating
FY2006	8,317,682	237,621	697,257	1,106,588	2,260,223	4,010,629	**16,630,000**
FY2007	8,628,287	245,640	712,875	1,133,159	2,322,556	3,997,483	**17,040,000**
FY2008	8,905,533	253,572	734,450	1,167,647	2,385,373	4,115,424	**17,562,000**

Table 7: Overhead, Escalation, and Other Rates used in Budget Estimates

Overhead Assumptions		FY06	FY07	FY08
	Escalation(per DOE)		1.7%	1.8%
	Wage pool escalation		3.0%	3.0%
	Materials escalation		2.0%	2.0%
	Utilites/Space escalation		3.0%	3.0%
	G&A (incl legacy)	37.9%	36.4%	36.4%
	Travel	7.0%	7.0%	7.0%
	Subcontract Tax	1.1%	1.1%	1.1%
	Award Fee	2.1%	2.1%	2.1%
	TN Use Tax (applied to materials)	7.0%	7.0%	7.0%
	Space rate/sq ft	22.08	22.74	23.42
	Utility rate/sq ft	17.28	17.80	18.33

The cost indicated for guests is an estimate of 50% of the salary/fringe cost for university professors. A FY06 base of 100K is assumed, plus 3% escalation for the out-years. With the assumption that this cost will be covered by a university subcontract, subcontract overhead rates have been assumed. Again, the Award Fee is charged against both the value of the subcontract and the subcontract overhead.

Travel: Travel budgets have been estimated at 3% of the fully burdened scientific staff cost. This methodology parallels that used by the Spallation Neutron Source. An alternate approach considered was to assume a fixed budget/number of trips per FTE supported. An assessment with this alternate approach supported the budgets determined by the method used. The average travel budget per scientific FTE is roughly $4,000 with some variations by scientific theme. For example, the travel budget per FTE in the administration/management office is $8,000 per FTE, which is appropriate given the role of this office in publicizing the CNMS. The travel budget for the neutron/x-ray staff is likewise close to $8,000 per FTE, very appropriate given the likely travel to other neutron and x-ray sources across the world.

ORNL has a special overhead rate for travel (see Table 7). The Award Fee is charged against both the cost of the travel and the travel overhead.

Maintenance: For each of the scientific theme areas, maintenance refers to upkeep of scientific equipment and instrumentation. Infrastructure/building maintenance is budgeted as part of the building support. Maintenance of major items of equipment (electron lithography, electron microscopes, etc.) will be through service subcontracts with the vendors. This is the standard approach for these instruments. Routine repairs will be performed by the hourly crafts from ORNL as appropriate. The budgeted amounts are estimated as a percentage of the fully burdened staff cost. Use of this basis is reasonable since the amount of equipment in a research effort is typically related to the number of staff required to operate it. The percentage of the staff cost varies with the kind of research. For the clean room and the on-site electron microscopes, the percentage is 20% due to the expensive service contracts as well as the amount of other maintenance activities required for these operations. For computational research and the administration offices this rate is set at 1%, an amount adequate for routine computer repairs. For all other research activities, this is set at 5%. These budgets were reviewed and validated by the scientific staff for each of the efforts and through benchmarking with similar clean room and microscopy activities.

Since much of maintenance is people costs, for simplicity the full ORNL G&A has been applied to the estimated cost. For subcontracted maintenance, the actual overhead would be less. Again, the award fee is charged against the sum of the maintenance and the G&A cost.

Materials/Consumables: Materials and consumable items include normal laboratory supplies, spares, chemicals, small equipment items, replacement computers, software/software licenses, office supplies, etc. This budget item also includes disposal of waste chemicals. Again, the budget estimates have been based on percentages of burdened staff salary costs. For the clean room and microscopes this percentage is 20%, recognizing the materials-intensive nature of these activities. For the clean room, spares, gowns, chemicals, etc. are major cost items. For other research activities, including computational research, this budget is set at 10% of the staff cost. For the computational area, the big expense is licensing fees and replacement computers. Again, the budget estimates were reviewed by the scientific leadership for the CNMS and deemed appropriate based on our existing laboratory experience. Clean room expenses were validated in comparison to similar clean room operations at other institutions.

Operating and Capital Budgets: FY 2006, 2007, and 2008 (continued)

In Tennessee, the cost of materials is taxed at the State Use Tax rate (see Table 7). There are also some local taxes that are applied, but this is a negligible cost for these estimates. G&A overhead is applied to the first 35,000 of any individual purchase (but is not applied to use tax). Finally, the Award Fee is charged on the total cost including use tax and overheads.

Building Support: At ORNL, maintenance of the building infrastructure and utilities are charged out on a per square foot basis for the space occupied by laboratories and offices. Space charge is not levied against lobbies, common spaces (e.g., restrooms, stairwells, etc.), and non-research service space (e.g., utility rooms). The estimated rates for these activities are included in Table 7 above. In the calculations, it has been assumed that CNMS will receive space/utility charges on 45,000 of the 48,000 net square feet of the facility. The estimated requirements for building support are summarized in Table 8.

Also included as building support are estimated charges for telephones and IT lines. These are based on the rates currently included in the FY06 budgets for ORNL. Finally, a miscellaneous category has been included to cover a host of minor charges typically assessed for common functions. The values used here are based on what is typically seen at ORNL in research organizations.

A final note: ORNL typically charges out building support and general administration costs (including ESH, clerical support, etc.) as an hourly charged rate for staff time that goes to programs. For the purposes of this budget review, the detail of what makes up these charges has been listed. The cost to the CNMS is the same, whether charged directly or as part of an organizational burden rate. Full G&A and award fee rates are applied to these costs.

Table 8: Building Support Budgets for FY2006, 2007 and 2008

Building Support Summary	FY2006		FY 2007		FY2008	
	no overhead	with overhead	no overhead	with overhead	no overhead	with overhead
Space/utilities: 45,000 sq ft	1,771,200	2,493,777	1,824,336	2,540,651	1,879,066	2,616,870
Telecom. (phone + comp)	239,023	336,535	240,720	335,237	241,082	335,742
Misc.	250,000	351,990	257,500	358,606	265,225	369,364
Total	2,260,223	3,182,301	2,322,556	3,234,494	2,385,373	3,321,976

Capital Equipment: Capital equipment is essential for the CNMS. With the current operating budgets these funds are significantly constrained. The amounts budgeted for each year are shown in Table 9. Table 10 shows the distribution of capital and operating funds for each year. Capital is about 10% of the total funding in FY2006 and FY2007, but begins to drop in FY2008 because the escalation provided in the total budget guidance is less than the 3% anticipated escalation in salary/fringe and utility/building costs. Note that had the ORNL G&A rate not dropped in FY2007, this effect would have been seen that year as well.

Table 9: Budgeted Capital Equipment by Year

Cost Summary	**Capital Equipment**	**ORNL OHs/Use Tax**	**Total Capital Equipment**
FY2006	1,683,703	186,297	**1,870,000**
FY2007	1,754,858	205,142	**1,960,000**
FY2008	1,743,628	194,372	**1,938,000**

Table 10: Budget Distribution between Operating and Capital

Cost Summary		Total Operating	Total Capital Equipment	Total
	FY2006	**16,630,000**	**1,870,000**	**18,500,000**
	FY2007	**17,040,000**	**1,960,000**	**19,000,000**
	FY2008	**17,562,000**	**1,938,000**	**19,500,000**

The details for potential equipment purchases are listed in the information for each scientific theme that is provided in section III.4 below. One item of particular note is the inclusion of approximately $500K per year to support the ORNL Center for Computational Sciences. This amount will insure CNMS users access to the best computational resources and expertise in facilitating use of the computer and adapting codes to effectively utilize it.

If additional budget were to become available then additional capital equipment for ongoing renewal of unique and state-of-the-art capabilities would be a very high priority. In addition, beginning in FY2009, we are requesting that DOE-BES provide the equivalent of "Accelerator Improvement Project" (AIP) funding to provide replacement of major user instrumentation. Assuming a 5-year technology lifetime for the leading instrumentation, the budget needs in this category *will far exceed* what can be accomplished with normal capital funding resources. The funding in this category is estimated to be $3M per year, with occasional increases to the $5 to 6M level for a given year to upgrade single instruments whose cost is in this range.

In Tennessee, the cost of all materials, including capital equipment, is taxed at the State Use Tax rate (see Table 7). Some local taxes also are applied, but this is a negligible cost for these estimates. G&A overhead is applied to the first 35,000 of any individual purchase (but is not applied to use tax). Finally, the Award Fee is charged on the total cost including use tax and overheads.

III.3 Staffing and Budget Summaries for Scientific Themes

Table 11 summarizes the staffing detail for each of the Scientific Themes by fiscal year. Note that all administrative staff and the long-term guests, except those associated with the Nanomaterials Theory Institute, are shown with the Management and Administration section.

Table 11: Staffing Comparison for Scientific Themes by Fiscal Year

Cost Summary: FY2006		Sci FTEs	Support FTEs	Postdoc FTEs	Guest FTEs	Staff Cost
	Management and Adminsitration	2.5	7	0	6	1,732,407
	Macro Systems	3.4	2	5	0	919,882
	Func Nanomaterials	3.55	1	5	0	892,279
	Magnetism & Transport	1.5	0	3	0	413,513
	Catalysis	2.8	0.8	2	0	575,323
	Nanotheory Institute	4.25	1	4	3	1,338,970
	Nanofabrication Research Lab	3.7	8.25	3	0	1,275,965
	Nanoscale Imaging,Char & Mar	4.7	3.9	3	0	1,169,343
	Total	**26.40**	**23.95**	**25.00**	**9.00**	**8,317,682**

Cost Summary: FY2007		Sci FTEs	Support FTEs	Postdoc FTEs	Guest FTEs	Staff Cost
	Management and Adminsitration	2.75	7	0	6	1,845,455
	Macro Systems	3.4	2	5	0	947,478
	Func Nanomaterials	3.55	1	5	0	919,047
	Magnetism & Transport	1.5	0	3	0	425,919
	Catalysis	2.8	0.8	2	0	592,582
	Nanotheory Institute	4.25	1	4	3	1,379,139
	Nanofabrication Research Lab	3.7	8.25	3	0	1,314,243
	Nanoscale Imaging, Char, & Ma	4.7	3.9	3	0	1,204,424
	Total	**26.65**	**23.95**	**25.00**	**9.00**	**8,628,287**

Cost Summary: FY2008		Sci FTEs	Support FTEs	Postdoc FTEs	Guest FTEs	Staff Cost
	Management and Adminsitration	2.75	7	0	6	1,919,914
	Macro Systems	3.4	2	5	0	975,942
	Func Nanomaterials	3.55	1	5	0	946,619
	Magnetism & Transport	1.5	0	3	0	438,696
	Catalysis	2.8	0.8	2	0	610,360
	Nanotheory Institute	4.25	1	4	3	1,419,774
	Nanofabrication Research Lab	3.7	8.25	3	0	1,353,671
	Nanoscale Imaging, Char, & Ma	4.7	3.9	3	0	1,240,556
	Total	**26.65**	**23.95**	**25.00**	**9.00**	**8,905,533**

Staffing and Budget Summaries for Scientific Themes (continued)

Table 12 summarizes the total budget by area for each fiscal year. In the subsequent section, the detailed staffing and budgets for the Management and Administration and for each Scientific Theme area are provided, including a listing of potential capital items.

Table 12: Budget Comparison for Scientific Themes by Fiscal Year

Cost Summary: FY2006	Staff Cost	Travel	Maintainance	Consumables/ Materials	Building Support	ORNL OHs/Use Tax	Total Operating	Capital Equipment	ORNL OHs/Use Tax	Total Capital Equipment	Total
Management and Adminsitration	1,732,407	40,652	22,137	66,412		527,743	**2,389,351**	NA			**2,389,351**
Macro Systems	919,882	28,322	57,215	114,429		308,331	**1,428,179**	380,000	48,682	**428,682**	**1,856,862**
Func Nanomaterials	892,279	30,402	55,675	111,351		303,153	**1,392,860**	0	0	**0**	**1,392,860**
Magnetism & Transport	413,513	14,412	24,019	48,038		102,334	**602,316**	0	0	**0**	**602,316**
Catalysis	575,323	19,700	36,838	73,676		215,607	**921,144**	0	0	**0**	**921,144**
Nanotheory Institute	1,338,970	45,032	16,235	162,351		377,565	**1,940,154**	445,280	54,719	**499,999**	**2,440,153**
Nanofabrication Research La	1,275,965	26,143	342,167	342,167		750,190	**2,736,632**	0	0	**0**	**2,736,632**
Nanoscale Imaging, Char, &	1,169,343	32,957	142,970	188,164		503,628	**2,037,062**	750,000	82,896	**832,896**	**2,869,958**
Support Costs											
Space/utilities: 45,000 sq ft					1,771,200	722,577	**2,493,777**				**2,493,777**
Telecom. (phone + comp)					239,023	97,512	**336,535**				**336,535**
Misc.					250,000	101,990	**351,990**	108,423		**108,423**	**460,413**
Total	**8,317,682**	**237,621**	**697,257**	**1,106,588**	**2,260,223**	**4,010,629**	**16,630,000**	**1,683,703**	**269,193**	**1,870,000**	**18,500,000**

Cost Summary: FY2007	Staff Cost	Travel	Maintainance	Consumables/ Materials	Building Support	ORNL OHs/Use Tax	Total Operating	Capital Equipment	ORNL OHs/Use Tax	Total Capital Equipment	Total
Management and Adminsitration	1,845,455	44,176	23,473	70,420		549,688	**2,533,211**	NA			**2,533,211**
Macro Systems	947,478	28,979	58,497	116,994		305,457	**1,457,405**	0	0	**0**	**1,457,405**
Func Nanomaterials	919,047	31,091	56,918	113,836		300,328	**1,421,220**	0	0	**0**	**1,421,220**
Magnetism & Transport	425,919	14,766	24,610	49,221		101,444	**615,960**	850,000	91,607	**941,607**	**1,557,567**
Catalysis	592,582	20,131	37,631	75,262		213,565	**939,172**	115,000	24,178	**139,178**	**1,078,350**
Nanotheory Institute	1,379,139	46,108	16,617	166,165		374,744	**1,982,773**	445,000	54,157	**499,157**	**2,481,929**
Nanofabrication Research Lab	1,314,243	26,705	349,069	349,069		741,719	**2,780,805**	0	0	**0**	**2,780,805**
Nanoscale Imaging, Char, & M	1,204,424	33,684	146,059	192,191		498,602	**2,074,960**	240,000	35,200	**275,200**	**2,350,161**
Support Costs											
Space/utilities: 45,000 sq ft					1,824,336	716,315	**2,540,651**				**2,540,651**
Telecom. (phone + comp)					240,720	94,517	**335,237**				**335,237**
Misc.					257,500	101,106	**358,606**	104,858		**104,858**	**463,464**
Total	**8,628,287**	**245,640**	**712,875**	**1,133,159**	**2,322,556**	**3,997,483**	**17,040,000**	**1,754,858**	**205,142**	**1,960,000**	**19,000,000**

Cost Summary: FY2008	Staff Cost	Travel	Maintainance	Consumables/ Materials	Building Support	ORNL OHs/Use Tax	Total Operating	Capital Equipment	ORNL OHs/Use Tax	Total Capital Equipment	Total
Management and Adminsitration	1,919,914	46,093	24,375	73,124		567,216	**2,630,721**	NA			**2,630,721**
Macro Systems	975,942	29,850	60,255	120,510		314,640	**1,501,197**	0	0	**0**	**1,501,197**
Func Nanomaterials	946,619	32,024	58,625	117,251		309,338	**1,463,856**	635,000	71,726	**706,726**	**2,170,582**
Magnetism & Transport	438,696	15,209	25,349	50,698		104,487	**634,439**	0	0	**0**	**634,439**
Catalysis	610,360	20,735	38,760	77,520		219,972	**967,347**	0	0	**0**	**967,347**
Nanotheory Institute	1,419,774	47,460	17,105	171,047		385,639	**2,041,025**	445,000	54,157	**499,157**	**2,540,182**
Nanofabrication Research Lab	1,353,671	27,507	359,541	359,541		763,971	**2,864,230**	600,000	68,490	**668,490**	**3,532,719**
Nanoscale Imaging, Char, & M	1,240,556	34,695	150,441	197,957		513,560	**2,137,209**	0	0	0	**2,137,209**
Support Costs											
Space/utilities: 45,000 sq ft					1,879,066	737,804	**2,616,870**				**2,616,870**
Telecom. (phone + comp)					241,082	94,660	**335,742**				**335,742**
Misc.					265,225	104,139	**369,364**	63,628		**63,628**	**432,992**
Total	**8,905,533**	**253,572**	**734,450**	**1,167,647**	**2,385,373**	**4,115,424**	**17,562,000**	**1,743,628**	**194,372**	**1,938,000**	**19,500,000**

III.4 Staffing and Budget Details for Individual Scientific Themes

CNMS Management and Administration

Director's Office

Doug Lowndes (1.0)
Clerical/web support - Sandy Lowe (1.0)

Linda Horton (0.5); increased to 0.75 in FY 2007
Clerical Support (DD + staff) (2.0)
ESH – tbd (part of SNS staff; one in building and others with SNS) (2.0)
Note to extend operations beyond 12/5, additional ESH staff will be required
Financial support (0.5 with SNS)

User Coordinator's Office

Tony Haynes (1.0)
User Support – tbd (1.5) (0.5 with SNS, 1 located in CNMS)

Long-Term Guests (6)

Budget Summary by Fiscal Year:

Summary	Sci FTEs	Support FTE	Postdoc FTEs	Guest FTEs	Staff Cost	Travel	Maintain.	Consumables/Materials	ORNL OHs/Use Tax	Total Operating	Total
Management and Adminsitration											
FY 2006	2.5	7	0	6	1,732,407	40,652	22,137	66,412	527,743	**2,389,351**	**2,389,351**
FY 2007	2.75	7	0	6	1,845,455	44,176	23,473	70,420	549,688	**2,533,211**	**2,533,211**
FY 2008	2.75	7	0	6	1,919,914	46,093	24,375	73,124	567,216	**2,630,721**	**2,630,721**

Assumptions:
Travel: 3% of burdened staff costs
Maintenance: 1% of burdened scientific staff costs
Consumable Materials: 3% of burdened staff costs

Note: Except for those associated with the Nanomaterials Theory Institute, the budget for long-term guests is part of Management and Administration budget shown above. This is to insure that these valuable positions are not perceived as an entitlement by any of the scientific groups. Selection of these staff will be competitive and will be placed to insure maximum value to the User Program.

Staffing and Budget Details for Individual Scientific Themes (continued)

Macromolecular Complex Systems (Britt)

RFAs: *Synthetic and Bio-Inspired Macromolecular Materials* (Britt, Mays)
Nanophase Biomaterial Systems (Simpson, Doktycz)

Scientific Leadership:
Jimmie Mays (0.1), Phil Britt* (0.5), Mike Simpson* (0.1), Mitch Doktycz (0.1)

K. Hong (1.0)
TBD (0.6)
TBD (1.0)

3.4 FTEs (see above) plus
2 technical support staff (2.0)
5 postdocs

Budget Summary by Fiscal Year:

Summary	Sci FTEs	Support FTE	Postdoc FTE	Staff Cost	Travel	Maintain.	Consumables/Materials	ORNL OHs/Use Tax	Total Operating
Macro Systems									
FY 2006	3.4	2	5	919,882	28,322	57,215	114,429	308,331	**1,428,179**
FY 2007	3.4	2	5	947,478	28,979	58,497	116,994	305,457	**1,457,405**
FY 2008	3.4	2	5	975,942	29,850	60,255	120,510	314,640	**1,501,197**

Assumptions:
Travel: 3% of burdened staff costs
Maintenance: 5% of burdened scientific staff costs
Consumable Materials: 10% of burdened staff costs

Capital Equipment:
FY 2006 Suite of advanced polymers characterization instrumentation $428,682
FY 2007 None
FY 2008 None

Staffing and Budget Details for Individual Scientific Themes (continued)

Functional Nanomaterials (Geohegan, Christen)

RFAs: *Nanotubes, Nanowires, Quantum Dots, and Related Structures* (Geohegan, Lowndes)
Artificial Oxide Film Structures (Christen, Rouleau)

Scientific Leadership:
Dave Geohegan (0.5)/ Doug Lowndes*, Hans Christen* (0.3)

Phil Britt* (0.1)
TBD or Alex Puretzky (1.0)
TBD or Ilia Ivanov (0.6)
TBD or Zhengwei Pan (0.75)
TBD or Chris Rouleau (0.3)

3.55 FTE (see above) plus
1 technical support
5 postdocs

*Also listed under another Scientific Theme or area

Budget Summary by Fiscal Year:

Summary		Sci FTEs	Support FTE	Postdoc FTEs	Staff Cost	Travel	Maintain.	Consumables/Materials	ORNL OHs/Use Tax	Total Operating
	Functional Nanomaterials									
	FY 2006	3.55	1	5	892,279	30,402	55,675	111,351	303,153	**1,392,860**
	FY 2007	3.55	1	5	919,047	31,091	56,918	113,836	300,328	**1,421,220**
	FY 2008	3.55	1	5	946,619	32,024	58,625	117,251	309,338	**1,463,856**

Assumptions:
Travel: 3% of burdened staff costs
Maintenance: 5% of burdened scientific staff costs
Consumable Materials: 10% of burdened staff costs

Capital Equipment:

FY 2006 None
FY 2007 None
FY 2008 Pulsed laser system for ultra-thick structured materials $706,726

Staffing and Budget Details for Individual Scientific Themes (continued)

Nanoscale Magnetism and Transport (Plummer**, Baddorf**)

RFAs: *Magnetism in Nanostructured Materials* (Shen, Baddorf)
Quantum Transport in Nanostructured Materials (Baddorf, Kalinin, Pantelides)
Artificial Oxide Film Structures (Baddorf)

Scientific Leadership:
Ward Plummer* (0.2), J Shen (0.3), A Baddorf* (0.4)

TBD or Zheng Gai* (0.3)
TBD or An-Ping Li* (0.3)

1.5 FTEs (see above) plus
Technical support listed under Nanoscale Imaging, Characterization, and Manipulation:
UHV Scanning Probes
3 FTEs postdocs

* also listed under another Scientific Theme

Budget Summary by Fiscal Year:

Summary		Sci FTEs	Support FTEs	Postdoc FTEs	Staff Cost	Travel	Maintain.	Consumables/Materials	ORNL OHs/Use Tax	Total Operating
	Magnetism & Transport									
	FY 2006	1.5	0	3	413,513	14,412	24,019	48,038	102,334	**602,316**
	FY 2007	1.5	0	3	425,919	14,766	24,610	49,221	101,444	**615,960**
	FY 2008	1.5	0	3	438,696	15,209	25,349	50,698	104,487	**634,439**

Assumptions:
Travel: 3% of burdened staff costs
Maintenance: 5% of burdened scientific staff costs
Consumable Materials: 10% of burdened staff costs

Capital Equipment:
FY 2006 None
FY 2007 High Field, Low T Scanning Probe $941,607
FY 2008 None

Staffing and Budget Details for Individual Scientific Themes (continued)

Catalysis and Nano-Building Blocks (Overbury, **Schwartz**)

RFA: *Nanostructured Materials for Highly Selective Catalysis* (Overbury, Dist Sci TBD)

Scientific Leadership:
Steve Overbury (0.2); Dist Sci TBD (0.2)

Viviane Schwartz (1.0)
Hans Christen* (0.2)
Sergei Kalinin* (0.2)
TBD – (chemist) (1.0)

2.8 FTEs (see above) plus
0.8 technical support (0.3 not in CNMS building)
2 postdocs

*also listed under another Scientific Theme

Budget Summary by Fiscal Year:

Summary		Sci FTEs	Support FTEs	Postdoc FTEs	Staff Cost	Travel	Maintain.	Consumables/Materials	ORNL OHs/Use Tax	Total Operating
	Catalysis									
	FY 2006	2.8	0.8	2	575,323	19,700	36,838	73,676	215,607	**921,144**
	FY 2007	2.8	0.8	2	592,582	20,131	37,631	75,262	213,565	**939,172**
	FY 2008	2.8	0.8	2	610,360	20,735	38,760	77,520	219,972	**967,347**

Assumptions:
- Travel: 3% of burdened staff costs
- Maintenance: 5% of burdened scientific staff costs
- Consumable Materials: 10% of burdened staff costs

Capital Equipment:

FY 2006 None
FY 2007 Combinatorial Synthesis of Catalysts $139,178
FY 2008 None

Staffing and Budget Details for Individual Scientific Themes (continued)

Nanomaterials Theory Institute: Theory, Modeling, and Simulation (Cummings, Schulthess, Stocks**)**

RFAs: *Virtual Synthesis and Nanomaterials Design* (Cummings/Glotzer)
Electronic Structure, Correlations, and Transport in Nanostructured Materials *(*Schulthess/Stocks)

Scientific Leadership
Peter Cummings (0.25), NTI Steering Committee

Elbio Dagotto (UT Dist Sci new hire) (0.1)
TBD (UT Dist Sci new hire) (0.1)
Thomas Schulthess (0.2)
Malcolm Stocks (0.1)
TBD in support of NTI core functions (1.75)[i]
TBD in support of macromolecular/soft materials (0.5)[ii]
TBD in support of catalysis and nano-building blocks (0.25)[ii]
TBD or Meunier. Wells, Maier in support of Func Nanomaterial (0.5)[ii]
TBD or X. Zhang in support of quantum transport (0.5)[ii]

4.25 FTE (see above) plus
1 technical support
4 postdocs
3 FTEs long term university guests (NTI Visitors Program)

Note: **NTI Steering Committee** (~4 local and ~2 external; day-to-day operational guidance)
[i]on a yearly rotation along with long term university guests
[ii]on a longer rotation in sync with experimentally motivated RFAs

Budget Summary by Fiscal Year:

Summary		Sci FTEs	Support FTEs	Postdoc FTEs	Guest FTEs	Staff Cost	Travel	Maintain.	Consumables/Materials	ORNL OHs/Use Tax	Total Operating
	Nanomaterials theory Institute										
	FY 2006	4.25	1	4	3	1,338,970	45,032	16,235	162,351	377,565	**1,940,154**
	FY 2007	4.25	1	4	3	1,379,139	46,108	16,617	166,165	374,744	**1,982,773**
	FY 2008	4.25	1	4	3	1,419,774	47,460	17,105	171,047	385,639	**2,041,025**

Assumptions:
Travel: 3% of burdened staff costs
Maintenance: 1% of burdened scientific staff costs
Consumable Materials: 10% of burdened staff costs (includes licensing fees)

Capital Equipment and CCS Support:

FY 2006 CCS Support $500,000
FY 2007 CCS Support $500,000
FY 2008 CCs Support $500.000

Nanofabrication Research Laboratory (Simpson**/**TBD**, Kasica)**

Scientific Leadership
Mike Simpson* (0.2), TBD (0.5)

Rich Kasica (1.0)
TBD (1.0)
TBD (two @ 0.5)

3.7 FTEs (see above) plus
8 technical support staff (5 day operations/12 hours).
  Requires ramp-up period of employment for training before operation.
  2 e-beam staff and 5 for everything else
  1 technical support engineer to oversee common maintenance activities
3 postdocs
0.25 janitor support (balance of FTE for rest of building, incl in space charge)

Budget Summary by Fiscal Year:

Summary		**Sci FTEs**	**Support FTEs**	**Post doc FTE**	**Staff Cost**	**Travel**	**Maintain.**	**Consumables/Materials**	**ORNL OHs/Use Tax**	**Total Operating**
	Nanofabrication Research Lab									
	FY 2006	3.7	8.25	3	1,275,965	26,143	342,167	342,167	750,190	**2,736,632**
	FY 2007	3.7	8.25	3	1,314,243	26,705	349,069	349,069	741,719	**2,780,805**
	FY 2008	3.7	8.25	3	1,353,671	27,507	359,541	359,541	763,971	**2,864,230**

Assumptions:
  Travel: 3% of burdened staff costs
  Maintenance: 20% of burdened scientific staff costs
  Consumable Materials: 20% of burdened staff costs

Capital Equipment:
FY 2006 None
FY 2007 None
FY 2008 Soft Lithography Tools $668,490

Note: We are currently evaluating the FY06 staffing levels. Based on our recent benchmarking, it is likely that the final budget will show a 2-staff member reduction in technician staff for FY06 and a corresponding increase in the budget for consumable materials/maintenance associated with the initial operation of the clean room. The additional 2 technicians would be hired for FY07 when the user population is increasing.

Staffing and Budget Details for Individual Scientific Themes (continued)

Nanoscale Imaging, Characterization, and Manipulation:

Scientific Leadership:
UHV Scanning Probes: Ward Plummer* (0.1), **John Wendelken** (0.5)
Electron Microcopy and Spectroscopy: David Joy (0.25), Ian Anderson (0.3)
Neutron/x-ray scattering: Takeshi Egami (0.2), Mike Simonson (0.2)

TBD or Zheng Gai*	(0.7)
TBD or Minghu Pan	(0.75)
Mag staff (nano-SQUID/VSM/Andreev/sputter); TBD or An-Ping Li*	(0.65)
Art Baddorf* (Nanotransp System, except scanning probes)	(0.6)
Sergei Kalinin* (scanning probe instr devel + user training)	(0.2)
M. Varela – use of aberration corrected STEM	(0.25)
Larson/Ice - Affiliated	

4.7 FTEs (see above) plus
3.9 technical support (including instrument specialist (with SNS)
3 postdocs

*also in another Scientific Theme

Budget Summary by Fiscal Year:

Summary		Sci FTEs	Support FTEs	Post doc FTEs	Staff Cost	Travel	Maintain.	Consumables/Materials	ORNL OHs/Use Tax	Total Operating
	Nanoscale Imaging, Characterization, and Manipulation									
	FY 2006	4.7	3.9	3	1,169,343	32,957	142,970	188,164	503,628	**2,037,062**
	Fy 2007	4.7	3.9	3	1,204,424	33,684	146,059	192,191	498,602	**2,074,960**
	FY 2008	4.7	3.9	3	1,240,556	34,695	150,441	197,957	513,560	**2,137,209**

Assumptions:
- Travel: 3% of burdened staff costs
- Maintenance: 5% of burdened scientific staff costs (scanning probe), 20% (electron microscopes), 10% (neutron/x-ray scattering)
- Consumable Materials: 10% of burdened staff costs, 20% (electron microscopes)

Capital Equipment:

FY 2006	FE SEM	$832,896
FY 2007	None	
FY 2008	Dev of neutron environments	$ 275,200

IV. SCIENTIFIC IMPACT OF 10% ADDITIONAL BUDGET: Recommendations of the Scientific Advisory Committee

IV.1 <u>Advice and Recommendations from the SAC</u>

The CNMS SAC was convened at the end of January to obtain their advice and recommendations regarding the proposed CNMS Staffing Plan and Budget. The draft review document was sent to them by express mail and e-mail attachment on Jan. 30. A two-hour telephone conference call SAC meeting was held on Feb. 4 with all but one SAC member participating.

SAC members were asked to review the draft staffing plan and budget and then provide their advice and recommendations, while being guided by the following four questions:

(1) Are the numbers and types of positions and facilities adequate to reliably and safely address user research needs in a world-class nanoscience user research center?

(2) Are there appropriate concentrations of unique facilities and expertise to produce major advances in nanoscale scientific understanding (and ultimately nanotechnology)?

(3) Are we investing enough to continuously refresh a state-of-the-art Nanoscale Science Research Center?

(4) Are there other emerging scientific opportunities in which CNMS should play a role because of the available synergies and capabilities?

Near the close of the SAC meeting Dr. Jack Crow (the SAC Chair) summarized their answers to these questions, which are given at the end of this section. First, however, we present a brief digest of the SAC's discussion and responses on a number of important issues, paraphrasing their language wherever possible.

SAC members commented on and discussed a number of the Guiding Principles and Assumptions that are presented in section II of this document. Among their most strongly held beliefs were the following:

- There is a need for CNMS (and other NSRCs) to protect the staff's personal research time, which at CNMS is nominally only 15% (section II.4, Reliability of Operation and User Metrics). A statement should be made that "We fully recognize that part of the user support for research staff members will grow into collaborative research leading to joint publications."
- The CNMS investment in 10% of the salary of a number of leading scientists (section I.4.a, Scientific Themes) to guide its Scientific Themes—by encouraging user research at CNMS, organizing conferences and workshops, and mentoring students and postdocs—is good value, because CNMS is likely to obtain much more than 10% of their time.
- The breadth provided by CNMS initial Scientific Themes and staffing plan is important and *should not be narrowed any further* than already done due to budget constraints. Breadth in the initial scientific offerings and in leadership expertise is needed to bring users, many of whom will provide different and complementary expertise. The real opportunity for optimization of the CNMS scientific program will come after a few years experience, when it can be *scientifically guided* by the known strengths of CNMS and the still unknown strengths of its users. To try to guess these now may be foolish.

- The ORNL cost escalation numbers are marginally low, and DOE guidance is even lower.

SAC members also expressed serious and strongly stated concerns regarding specific CNMS scientific opportunities and needs that could and should be pursued if 10% additional base budget becomes available:

- There is a critical need for capital reinvestment to *sustain* CNMS as a state-of-the-art nanoscale science research center. CNMS is capital-poor because of budget constraints. *Renewal* must be a normal, ongoing part of operations: "If you cannot do this, then you are degrading." You can't wait 3–5 years to start renewing.
- Furthermore, staff levels grow in proportion to capital reinvestment. There's not enough capital reinvestment, or incremental personpower to go with it, to stay viable at the cutting edge.
- *Reinvestment for sustainability* is crucial for the NSRCs, and is an excellent investment. The marginal scientific productivity per additional dollar is huge: you're on the steep part of the productivity curve.
- Theory, modeling, and simulation (computational nanoscience) should be strengthened because this area is becoming a major strength for ORNL, allowing CNMS to have great scientific impact at the national level.
- Specific opportunities for CNMS to utilize neutron scattering at the SNS were discussed briefly, and include studies of magnetic multilayers/films and of the emergence of functionality through self-assembly of soft materials.

Dr. Crow's brief summary of the SAC's answers to the four questions that guided their discussion was as follows:

(1) Are the numbers and types of positions and facilities adequate to reliably and safely address user research needs in a world-class nanoscience user research center?
They are adequate for startup but staffing is tight.

(2) Are there appropriate concentrations of unique facilities and expertise to produce major advances in nanoscale scientific understanding (and ultimately nanotechnology)?
Yes, and this is adequately addressed in the review document.

(3) Are we investing enough to continuously refresh a state-of-the-art Nanoscale Science Research Center?
Capital investment is minimal because of budgetary constraints, and as the user program grows there will be significant staffing pressures.

(4) Are there other emerging scientific opportunities in which CNMS should play a role because of the available synergies and capabilities?
This could only be done by giving up existing Scientific Themes, due to budget pressure. However, SAC members support the CNMS' plan to maintain flexibility by periodically reviewing its scientific directions with the SAC.

Regarding both questions 3 and 4, the Chair's summary noted that both the CNMS' ability to continuously refresh its state-of-the-art capabilities, and its flexibility to pursue emerging scientific opportunities, are overly constrained by budget guidance.

(Please also see in Appendix D the letter dated Feb. 10 sent by Dr. Crow to Doug Lowndes.)

IV.2 **<u>CNMS Proposal for 10% Additional Base Budget</u>**

Based on our discussion with the SAC—particularly their comments about the need for initial breadth and for state-of-the-art sustainability—and keeping in mind ORNL strengths in neutron scattering and leadership computation, which can become unique assets for the national nanoscience community, CNMS proposes to invest 10% additional base budget ($1.85M yearly) entirely for the purpose of *ensuring state-of-the-art sustainability* at critical frontiers of nanoscale research, as follows:

1. Invest **$600K** to develop sample environments for nanoscience investigations using neutron scattering. This investment helps to rebuild the U.S. neutron scattering community and is an early opportunity for world leadership by BES in utilizing neutron scattering for nanoscale science. About $450K of this would be "seed" investment in capital equipment to encourage national collaborative teams to develop the new experimental environments, with additional equipment funding coming from proposals submitted to funding agencies by these teams. The balance would be used to support workshops to bring together and form the teams, and for CNMS research staff participation in the teams.

2. Invest **$500K** to support theory, modeling, and simulation activities of users at the *Nanomaterials Theory Institute* and utilizing the resources of ORNL's *Center for Computational Sciences*. Staff support for users will be the top priority.

3. Invest **$750K** in capital equipment needed to *ensure sustainability* at the state-of-the-art and *provide some flexibility* in pursuing emerging scientific opportunities. The focus here will be on delivering unique instruments to the nanoscience user community, as outlined in section I.4.b.

We recognize the SAC's concern about staffing levels in the out-years as the user program grows, and the possibility that some (ideally all) areas will prove very popular with users. We plan to re-evaluate staffing needs for all areas and adjust accordingly, including the application of some of the 10% additional base budget, as required.

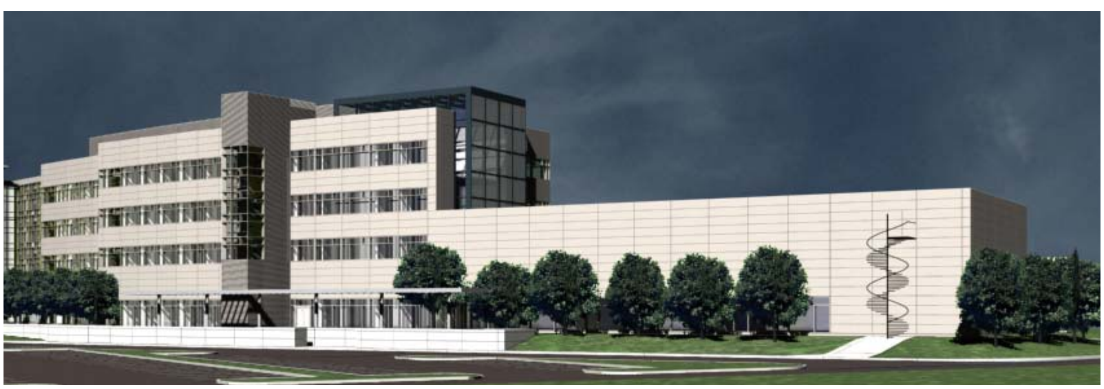
Together with the SAC, we believe that these are the key areas in which investments at CNMS will have maximum scientific impact, year after year, by utilizing unique ORNL strengths and making them accessible to the national nanoscience user community.

Appendix A
CNMS Building and Laboratories

The CNMS will be housed in an 80,000 sq foot building that is under construction on the Spallation Neutron Source site at ORNL (see Figure A1). Construction on the facility began in 2003 with anticipated completion in April 2005. As shown in Figure A2, the facility includes a four-level main building with wet and dry laboratories, office space, and common areas to promote interaction among staff, guests, and users. The 10,000 sq ft Nanofabrication Research Laboratory is housed on the ground level in a one-story wing of the building. It includes clean rooms as well as an area designed to meet the requirements of electron beam imaging and writing instruments (low electromagnetic fields, low vibrations, and low acoustic noise).

Figure A1: On the left, an aerial photo onto which the drawings of the SNS and the CNMS have been superimposed. On the right, an enlargement of the architect's rendition of the CNMS and the connection to the SNS Central Laboratory and Office Building.

Figure A2: Architectural drawing of the CNMS. The clean room is in the one-story wing; the balance of the laboratories, offices, and interaction space is in the four-story portion.



The CNMS will house up to 190 people in a combination of single-, double- and cubical occupancy. The labs in the 4-story portion are arranged in 20' x 25' modules that can be single-module labs or combined for a two-module 40' x 25' lab. There are 32 single-module labs in the building design.

The schematic in Figure A3 shows the ground floor of the CNMS. The clean room (numbered 1) is on the right side of the schematic. The left side shows the arrangement of the laboratories and offices in the 4-story portion of the building. The ground floor labs mainly house vibration-sensitive instrumentation and heavy equipment. (A pit for a STM has been added to the laboratory on the far left, resulting in a second lab with a double-module configuration) Note that the offices (numbered 4) are opposite the laboratories (numbered 5) and that the cubical space is centrally located adjacent to the private/2-person offices on the perimeter. This design maximizes interactions between users and staff. The Lobby (numbered 3) includes a conference area and open space for interactions and displays. Figures A4 and A5 show additional clean room details.

Figure A3: Schematic of the ground floor of the CNMS.

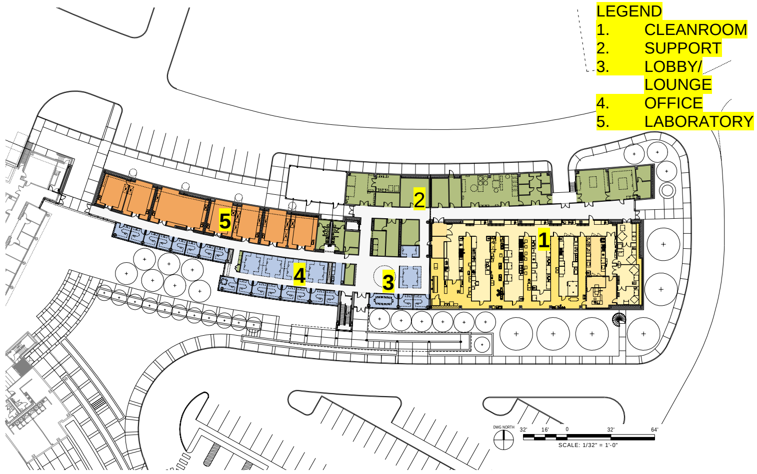
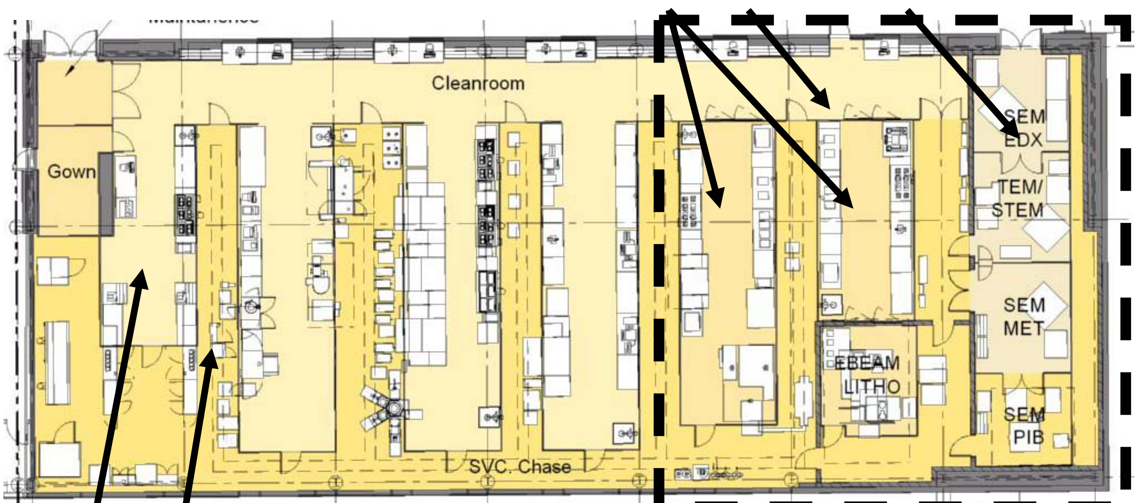


Figure A4: Schematic of the clean room area showing the cleanliness classifications of the areas and the area designated for sensitive equipment

Class 100, 1000, & 100,000 clean areas



Bay/chase configuration

Electromagnetic, vibration, acoustical (EVA) controlled area

Figure A5: Designation of the clean room areas by function

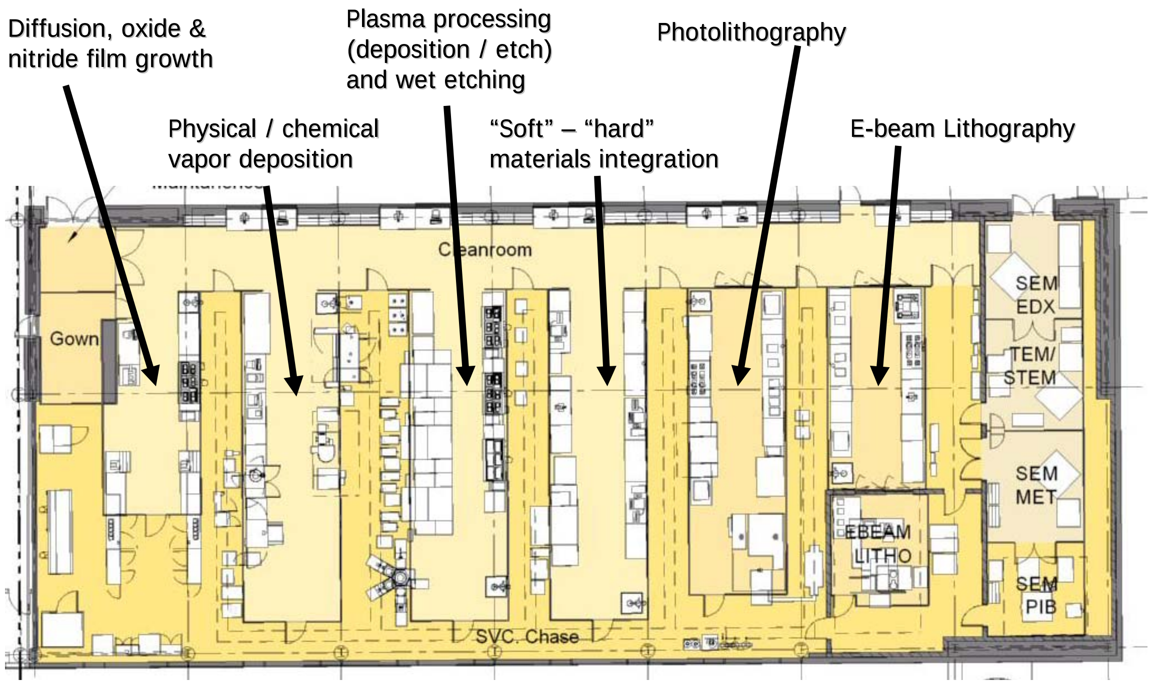
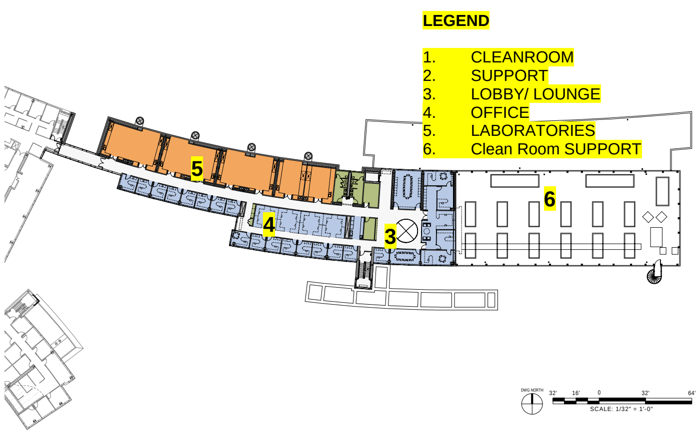


Figure A6: First Floor of the CNMS



The first floor of the CNMS, shown in Figure A6, houses additional laboratories, including laser synthesis laboratories. This floor is designed for heavier instrumentation than the other elevated levels. The management and administration area (offices surrounding the area labeled 3) is on this floor, as well as additional conference room and interaction spaces. Note that 3 of the laboratories on this floor are in the double-module configuration. These are laser synthesis and characterization laboratories.

The second floor, Figure A7, has all single-module laboratories. Included are 2 laboratories with provisions for up to 3 8-ft hoods. The area on the right side of the 4-story building will house the theory staff, including a large room for a computer with fiber connectivity to the Center for Computational Sciences on the main campus. The lobby area (labeled with a 3) has space for interactions and poster display. It is open through an atrium to the third floor and has lighting from sky lights. There is an additional conference room on this floor.

The top (third) floor is shown in Figure A8. All of the laboratories on this floor are equipped with 3 8-ft hoods. This is the focus of the wet chemistry synthesis in the CNMS. The offices on the right side of the building are for the theory effort. Again, there is a conference room and interaction space.

Figure A7: Schematic of second level of the CNMS

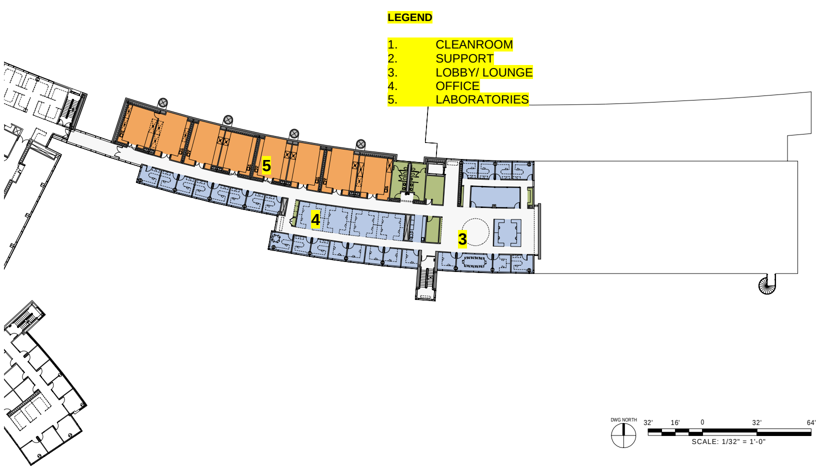
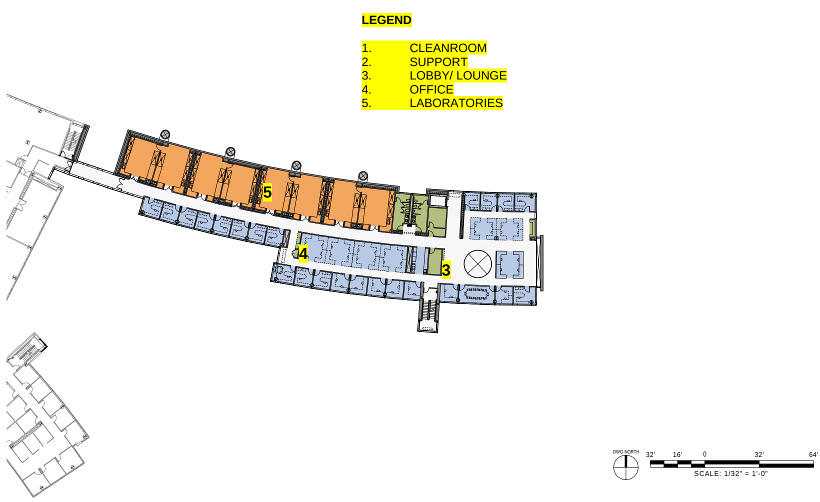


Figure A8: Schematic of third (the top) floor of the CNMS



Each of the laboratories in the 4-story portion of the CNMS has been designated a functional name. These are summarized in Table A1 below. In addition, shared scanning electron and transmission electron microscopes, as well as the Focused Ion Beam/SEM tool will be located in the sensitive-equipment area of the clean room. Computer equipment, including a Beowulf cluster, will be housed in the computer room on the second floor.

Table A1: List of laboratories, function, special equipment, and associated scientific theme for the laboratories in the 4-story CNMS

Floor	Designation	Special Equipment/Comments	Theme Area
Ground			
B8-B7	UHV Scanning Probes	Includes the pit for the "Ultimate STM"	Nanoscale Imaging, Characterization, and Manipulation
B6	Magnetic Materials Characterization	4-probe STM in SEM	Nanoscale Imaging, Characterization, and Manipulation
B5	Magnetic Materials Growth	Laser MBE	Nanoscale Magnetism and Transport
B4	Magnetic Imaging	SEMPA	Nanoscale Imaging, Characterization, and Manipulation
B3	Optical Characterization	AFM	Nanoscale Imaging, Characterization, and Manipulation
B2	Target Synthesis		Functional Nanomaterials
B1	Magnetic Characterization	Squid	Nanoscale Magnetism and Transport
First			
18–17	Pulsed Laser Deposition		Functional Nanomaterials
16–15	Laser Diagnostics/Characterization	Tunable Raman	Functional Nanomaterials
14–13	Laser Nanomaterials Synthesis	MOPO and YAG Laser Systems	Functional Nanomaterials
12	x-ray Diffraction Lab	x-ray Diffraction equipment	Nanoscale Imaging, Characterization, and Manipulation
11	Furnace Lab		General Support
Second			
28	Materials Synthesis	(3-hood lab)	Catalysis and Nano-building blocks
27	Materials Synthesis	(3-hood lab)	Catalysis and Nano-building blocks
26	Thermal Characterization	Polymer char. equip.	General Support
25	Laser-based characterization of soft materials	Elipsometer, Static and Dynamic Light Spect.	Macromolecular Complex Systems
24	Mass Spec Characterization	MALDI Time of Flight	General Support
23	Optical characterization	FTIR, UV-VIS	Macromolecular

			Complex Systems
22	NMR laboratory	Future NMR	Nanoscale Imaging, Characterization, and Manipulation
21	CVD		Functional Nanomaterials
38	Shared laboratory for synthesis	GPC, 3-hood lab	Macromolecular Complex Systems; Functional Nanomaterials
37	Bio-based synthesis	3-hood lab	Macromolecular Complex Systems
36	Composites lab	3-hood lab	Functional Nanomaterials
35	Inorganic Synthesis Lab	3-hood lab	Macromolecular Complex Systems; catalysis
34	Organometallic Lab	3-hood lab	Macromolecular Complex Systems
33	Block co-polymers	3-hood lab	Macromolecular Complex Systems
32	Free Radical Polymerization	3-hood lab	Macromolecular Complex Systems
31	Anionic Polymerization	3-hood lab	Macromolecular Complex Systems

Appendix B
Initial Technical Equipment Set

Table B1: Line Item Technical Equipment for the CNMS

Soft Materials Characterization
Gel Permeation Chromatography (GPC) and High Temperature GPC with Light Scattering Detector
UV–Vis Spectrophotometer
Fourier Transform Infrared Spectrometer (FTIR)
Matrix–assisted laser desorption/ionization time–of–flight mass spectrometer (MALDI–TOF–MS)-benchtop
Physical characterization of polymers: DSC
Surface Analysis Equipment: Ellipsometer
Simultaneous Static and Dynamic Light Scattering Spectrometer
Nanophase Materials Synthesis And Characterization Equipment
MOPO and YAG Laser Systems
Continuous Wave (CW) Ti-sapphire Ring Laser
Tunable Raman Spectrometer
4-probe transport Scanning Tunneling Microscope
High–resolution Spin–polarized Scanning Electron Microscope (SEMPA)
NanoFabrication Research Laboratory
Direct Write Electron Beam Lithography (DWEBL) System
Double–Sided Contact Mask Aligner and Wafer Bonder System
Laser Pattern Generator/Mask Writer
Electron Beam Lithography and Photolithography Resist Processing Equipment and development tools
Plasma Etching and Deposition Equipment
Oxidation, Annealing, Diffusion and Low Pressure Chemical Vapor Deposition Furnaces
Thin Film Processing Equipment
Metrology and Inspection Tools
Ancillary Equipment
Nanomaterials Theory Institute
32-node Beowolf Cluster
7 SGI Graphic Workstations
16 screen video wall
General Use Equipment
X–ray Diffraction Laboratory for Multi–User Nanoscience
Focused Ion Beam (FIB) / Scanning Electron Microscope (SEM) (Dual–Beam System)
Laboratory Fume Hoods, furnishings, misc. equip.
Furniture, personal computers, and data system equipment

APPENDIX C
General Policies and Procedures for User Access to the DOE Nanoscale Science Research Centers

1. Preamble

The mission of the Department of Energy (DOE) Nanoscale Science Research Centers (NSRCs) is to support users in doing outstanding science in a safe environment. To this end, each Center must have:

- An *array of state-of-the-art equipment and laboratories* for synthesis, fabrication, characterization, and simulation of nanoscale materials and structures
- A *skilled staff* to support this equipment, users, and the associated science and operations

but above all

- A *user scientific program* that provides leadership in nanoscale science and technology

This document addresses the policies and procedures for user access to the NSRCs.

2. Peer review and Advisory Bodies

The key to delivery of outstanding science is rigorous peer review that is fair, clear, expedient and sensitive to the needs of users. We envisage advisory committees of the following kind:

2.1 *Scientific Advisory Committee (SAC)*
Each Center will have a SAC or equivalent body that advises senior management on policies related to the optimization of the quality and quantity of the scientific productivity of the facility. The SAC will be composed of distinguished scientists from both inside and outside the nanoscale science community. Appointments to the SAC will be made by senior management based on nominations from the user community, the Center management, and its advisory bodies. The SAC will report to the Laboratory Director or Associate Laboratory Director with senior management oversight responsibility for the Center.

2.2 *Users' Executive Committee (UEC)*
Each Center will have a UEC or equivalent body that is elected by the user community at large. The UEC will serve as the official voice of the user community in its interactions with Center management. The UEC will elect its Chair and Vice-chair from among its own members, and the UEC Chair will automatically have an *ex officio* seat on the SAC.

2.3 *Proposal Review Committees (PRCs)*

Evaluation of General User (GU) proposals will be carried out by appropriately constituted Proposal Review Committees. The rank order of scores generated by the PRCs will be the primary input in the allocation of facility access to General Users. The PRC will also provide feedback to the investigators on the quality of their proposals and, where relevant, on perceived weaknesses. The PRC will consist of external scientists (without affiliation to the NSRC) with expertise in various research fields related to nanoscale research. Appointment to the PRCs will be made by the Center Director or designate based on nominations received from the user community and suggestions from the facility management. PRC subcommittees related to the Center's scientific thrusts may be appointed to ensure knowledgeable and efficient handling of user proposals.

3. Evaluation Criteria and Process

The evaluation criteria used in the peer review procedures will take as their starting point the criteria proposed by the International Union of Pure and Applied Physics (IUPAP) in its recommendations on the operation of major user facilities (http://www.iupap.org/statements.html#facil). These are:

- Scientific merit
- Technical feasibility
- Capability of the experimental group
- Availability of the resources required

These criteria may be supplemented with additional requests, for example to justify the need for special equipment or to satisfy safety and environmental concerns. Special consideration will be given to encourage and support first time users so they can compete effectively in the peer review system. Preference may be given to proposals that utilize the unique capabilities of a Center and contribute to its established scientific thrust areas. The paramount criterion will be scientific merit.

User proposals will be directed first to the Center for a feasibility and safety review. A proposal considered not feasible or safe will be returned to the proposer with appropriate comments including suggested changes.

4. Modes of User Access

To deliver outstanding science, there must be access modes that are sufficiently flexible so as to be responsive to user needs. There are two basic modes of user access, General User access and Partner access, each with variable scope.

4.1 *General User Access*

General Users are individuals or groups who need access to the facility to carry out their research, using existing equipment in the NSRCs. General Users apply for access by submission of a proposal that is evaluated by one of the PRCs. The scope of a General User proposal can vary from a single experiment proposal to a program proposal (valid for multiple visits and substantial access to a range of equipment extended over multiple years) to a “special” proposal (i.e. rapid access, feasibility studies, or other means which have been developed by each Center based on their particular needs). Individual and group proposals, including collaborative proposals with NSRC staff, are encouraged.

4.2 *Partner Access*

Partners are individuals or groups who not only carry out research at an NSRC but also enhance the capabilities or contribute to the operation of the Center. Typically they develop the facility instrumentation in some way, bringing outside financial and/or intellectual capital into the evolution of the NSRC, or contribute to the operation of equipment and facilities. These contributions must be made available to the General Users and so benefit them as well as the facility. In recognition of their investment of either resources or intellectual capital and in order to facilitate and encourage their involvement, Partners may be allocated limited access to one or more facilities over a period of several years, with the possibility of renewal. Partner scientific programs are subject to the same peer review process as General Users.

5. Proprietary and Non-Proprietary Research

Users of the facilities include academic, industrial and government scientists and engineers. While the vast majority of user research should be in the public domain, and so must be disseminated by publication in the open literature, there may be access for proprietary research that utilizes these unique facilities to benefit the national economy. Users conducting proprietary research may access the facility as either General Users or as Partners. Full cost recovery will be obtained for proprietary research, and efforts will be made to secure appropriate intellectual property control for proprietary users to permit them to exploit their experimental results.

6. User Access Allocation, Scheduling, and Recording

Allocation of access to equipment and facilities for General Users will be done based on the rankings provided by the PRCs. Partners will manage their own scientific programs, subject to PRC review, and will allocate access among their members. Scheduling of user access will be centralized in the facility User Office using expert input from facility staff and Partner representatives. Center management will have ultimate responsibility and accountability for effective and efficient utilization of time on all equipment at the facility.

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February 10, 2004

Dr. Douglas H. Lowndes, Scientific Director
Center for Nanophase Materials Sciences
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6056 USA

Re: Recommendations from the CNMS Scientific Advisory Committee- CNMS Staffing/Budget Plan

Dear Dr. Lowndes,

The CNMS Scientific Advisory Committee (SAC) convened in a conference call on February 4, 2004. Members of the SAC participating included Drs. Bernholc, Crow (Chair), El-Sayed, Horton, Mason, Smalley, Stocks and Weertman. A draft copy of the CNMS Operational Budget Review Proposal was express mailed to all the members of the SAC for their review along with a cover letter from Dr. D. Lowndes, Scientific Director, CNMS. In the cover letter, the SAC was charged to provide advice and guidance regarding the proposal and specifically requested to address four primary issues. This brief response from the SAC primarily focuses on the four issues raised in the cover letter.

1) Are the number and types of positions and facilities adequate to reliably and safely address users research needs in a world-class nanoscience user research center?

The current portfolio of scientific themes that had been developed through numerous workshops with the users community is well balanced and focused. A particularly strong aspect of the effort is the opportunity to make available unique sample environments specifically suited for nanoscience investigations using the neutron scattering facilities at the SNS and HFIR. Several instruments planned for the SNS, e.g., the reflectometers and small angle scattering capabilities, are particularly well suited for nanoscience and heavy demand is anticipated. Sample environment on these instruments should be available that adequately address the needs of this segment of the nanoscience users community. The current breadth of the scientific themes should not be narrowed further due to budget constraints. As the scientific and user programs develop, there will be a natural selection of those themes that provide the most excitement and user involvement. In anticipation of this, the CNMS is urged to develop a review process to track user involvement and scientific accomplishments. There should be a careful review of the scientific portfolio after a center has been in operation for a few years. Trying to re-evaluate the themes and develop priorities within the portfolio at this time is meaningless and would be a disservice to the Center and its users community that have worked so hard to develop the current vision.

The 10% salary support provided to a number of leading scientists to guide some of the scientific themes within the CNMS proposed program is a very good investment. These individuals bring strong scientific credentials to the program and their leadership in the earlier years of the program will help stimulate user involvement. The SAC feels this modest investment will lead to significant paybacks beyond the 10% invested. The proposed scientific program needs senior leadership and these individuals will provide it. As the Center matures, these leadership positions can be shifted to the next generation of scientific staff that will be developed around the Center.

The overall staffing and budget plan appears to be adequate, however, it should be recognized that it just meets minimal expectations. The CNMS and advisory bodies should carefully monitor the development of the themes and adjust staffing levels as user and scientific demand dictates. The cost escalation estimates contained in the budget may be marginal and Center growth should be carefully monitored.

2) Are there appropriate concentrations of unique facilities and expertise to produce major advances in nanoscale scientific understanding (and ultimately nanotechnology)?

The current staffing and budget plan is minimal but adequate at this time. The proposed concentration of state-of-the-art instrumentation has been developed with considerable advice from the user community and represents an excellent start. The CNMS staffing plan including the involvement of shared positions in senior leadership positions should provide the leadership to lead the Center as it further develops its scientific vision and goals and develops a world-class users program.

3) Are we investing enough to continuously refresh a state-of-the-art Nanoscale Science Research Center?

The SAC is deeply concerned that the proposed budget does not provide adequate recurring capital to re-invest in state-of-the-art instrumentation. It was generally agreed that the Center initial facilities plan will certainly put the Center in a leadership position but much of the instrumentation will continually need upgrades and will need to be augmented by other facilities as the user activities grow and new scientific opportunities emerge. DoE and the Center should carefully re-examine their commitment to re-capitalization. Reinvestment into the infrastructure and facilities needs to be a critical component to the long-term planning if the initial expectations for success of the DoE nanoscience program are to be met. Reinvestment for sustainability is crucial for the NSRCs and represents an essential investment.

4) Are there other emerging scientific opportunities in which CNMS should play a role because of the available synergies and capabilities?

The Center leadership in cooperation with the user community has developed a strong portfolio of scientific themes. As indicated above, the Center should focus in these areas but continue to maintain a vigil on the user commitment to the areas and the early achievements. A re-evaluation of the program and allocation of resources should be pursued after a few years of operation. However, the SAC does feel strongly that the theory, modeling and simulation, i.e., the computational nanoscience component to the Center's scientific agenda, should be strengthened. This area has the great potential in guiding and stimulating research in other areas and it builds on strengths at Oak Ridge National Laboratory. This is certainly an area where Oak Ridge could establish national leadership and a world-class capability.

Sincerely,

Jack E Crow

Jack E. Crow, Chair
CNMS SAC